Novel MINLP Formulations for Flexibility Analysis for Measured and Unmeasured Uncertain Parameters

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Abstract

In this work, we formulate the extended flexibility analysis, which takes into account two different types of uncertain parameters: measured (θ_m) and unmeasured (θ_u), as a rigorous multi-level optimization problem. We recursively reformulate the inner optimization problems by the KKT conditions and with a mixed-integer representation of the complementarity conditions to solve the resulting multilevel optimization problem. Special cases are identified, where models are comprised of convex constraints or constraints with monotonic variation of the uncertain parameters. In these cases, a vertex enumeration can be performed to solve the flexibility test. We propose two MINLP reformulations for the more general case yielding to similar results but different model sizes. The formulations are tested and compared with several examples.

Keywords

Flexibility Analysis, Optimization under Uncertainty, Mixed-Integer Nonlinear Programming.

1. Introduction

Traditionally, the approach to handle uncertainty in the parameters of a model is to consider nominal conditions in plant operation and use overdesign to compensate for the potential impact of the uncertainty. In contrast, flexibility analysis addresses the

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This paper is devoted to the memory of Professor Roger Sargent, pioneer and intellectual founder of Process Systems Engineering.

guaranteed feasibility of operation of a plant over a specified range of conditions, with the ultimate goal being on how to design a process for guaranteed flexible operation (Grossmann, Calfa and Garcia-Herreros 2014).

First, Grossmann and Sargent (1978) addressed the problem of optimal design with uncertain parameters. They represented the design problem under uncertainty as a two-stage programming problem of infinite dimensions in the uncertain parameters space, θ. To handle the problem, a discretization procedure was applied, resulting in a finite number of points in the space of θ. To solve the problem, the authors proposed a mathematical formulation strategy that led to a large NLP problem, where the inequality constraints were maximized with respect to the uncertain parameters. To overcome the difficulty of solving a large NLP problem, Grossmann and Halemane (1982) proposed a decomposition technique based on a projection-restriction strategy to exploit the block diagonal structure resulting of the mentioned representation of the problem.

Later, Halemane and Grossmann (1983) formally proved the rigorous mathematical formulation for the flexibility test problem for a fixed design d. They demonstrated the equivalence of the logic expression (1) and the max-min-max constraint (2) that involves a non-trivial optimization problem, whose objective is to ensure feasible operation over the entire range of variation of the uncertain parameters and accounting for the fact the control variables z are adjusted for every parameters value θ.

$$\forall\theta \in T \left\{\exists\, z\,, \forall\, j \in J\, \left[f_j(d,z,\theta) \le 0\right]\right\} \tag{1}$$

$$\max_{\theta\in T} \min_{z} \max_{j\in J} f_j(d,z,\theta) \le 0 \tag{2}$$

To simplify the solution of the max-min-max problem in the flexibility constraints, Swaney and Grossmann (1985) considered the case of convex inequalities, where the solution of the flexibility constraint can be shown to lie at one of the vertices of the uncertainty set $T = \{\theta|\theta^{LB} \le \theta \le \theta^{UB}\}$. It is then possible to solve a minimization problem, Eq. (3), at every vertex $v \in V$ and then compute the maximum constraint violation with Eq. (4).

$$\psi(d,\theta^v) = \min_{z,u}(u|f_j(d,z,\theta^v) \le u, j \in J) \tag{3}$$

$$\chi(d) = \max_{v \in V}\{\psi(d, \theta^v)\} \tag{4}$$

This method is able only to find vertex solutions, and scales exponentially with the number of uncertain parameters. Grossmann and Floudas (1987) proposed the Active Set Method (ASM) consisting of a bilevel optimization problem that allows the explicit solution of Eq. (2). The formulation is based on 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 given design.

$$\begin{gathered} \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta) \\ s.t.\;\; \psi(d, \theta) = \min_{z,u}(u | f_j(d, z, \theta) \le u, j \in J) \end{gathered} \tag{5}$$

Specifically, in the bilevel programming problem Eq. (5), the lower level optimization problem, $\psi(d, \theta)$, is replaced by its KKT optimality conditions, where the complementarity conditions are represented with mixed-integer constraints. It is important to note that this MILP/MINLP formulation does not rely on the assumption of critical points corresponding to vertices, nor is it required the exhaustive enumeration of vertex points.

Bandoni *et al.* (1994) proposed the worst-case algorithm (WC) consisting of two-level optimization strategy. The outer level is solved for fixed values of θ, whereas in the inner level the feasibility of the constraints is established by performing maximization of each constraint $j \in J$ for the optimal point found at the outer level (fixed values of control variables, z). The algorithm converges when there are no more violated constraints in the inner level. Later, Raspanti *et al.* (2000) improved the WC algorithm by aggregating the constraints using the KS function (Kreisselmeier and Steinhauser 1983), where the inner level problem is reduced to a single maximization problem. Based on these ideas, the authors proposed the single level worst case (SLWC) reformulation. In addition, they proposed modified versions of the ASM. The first modification involves the use the KS function, which is a smooth approximation to the non-differentiable maximization function, $\max_{j \in J} f_j(d, z, \theta)$. This replacement results in only one constraint for which there is no need to include complementarity conditions, and hence leads to a single level NLP problem. The second modification was the replacement of the mixed-integer representation of the complementarity constraints with smoothing functions, again resulting in an NLP problem. While the advantage of this approach is that it reduces the max-min-max problem to a single NLP, it has the limitations that it is nonconvex and does not preserve linearity if the inequalities f_j are linear.

Recently, Zhang *et al.* (2016) studied the flexibility analysis for linear systems and established the relationship between flexibility analysis and robust optimization. They also proposed the dual-based flexibility analysis, a new reformulation of the flexibility constraint, in which the lower level problem is replaced by its dual problem and binary variables are introduced to represent the vertices of the uncertainty set. Based on Zhang's work, Jiang *et al*. (2018) proposed and algorithm to solve flexibility analysis of quadratic problems inspired on the outer-approximation algorithm for convex mixed-integer nonlinear programming.

In most areas, the set of uncertain parameters is described by a hyperrectangle. However, in some situations, this may result in conservative estimates. Data availability allows a better definition of the uncertainty in a statistical sense, for example, by probability distribution functions. In these lines, Pistikopolous and Mazzuchi (1990) and Straub and Grossmann (1990) determined a stochastic flexibility index that measures the probability that a given design is feasible to operate for linear systems. An extension to nonlinear system was later introduced by Straub and Grossmann (1993). Recently, Terrazas-Moreno *et al.* (2010) proposed a new approach to calculate the expected stochastic flexibility. The uncertain parameter space is discretized, and the probability associated to each point is calculated. Feasibility is checked for every collocation point by introducing binary variables instead of using a bounding search procedure (Straub and Grossmann 1990).

Rooney and Biegler (1999) introduced a more accurate description of the model parameter uncertainty using discrete values based upon the principal components of their joint confidence regions, i.e. elliptical joint confidence regions. Then, the same authors (2001) improved the description of model parameter uncertainties using confidence regions derived from the likelihood ratio test. More recently, Pulsipher and Zavala (2018) studied the case where the uncertainty set is characterized by multivariate Gaussian random variables and the model constraints are linear, yielding a mixed-integer conic programming (MICP) formulation for the flexibility index. In addition, they demonstrated that the flexibility index can be used to obtain a lower bound for the stochastic flexibility index (Straub and Grossmann 1990).

Flexibility analysis of dynamic systems has been addressed by Dimitriadis and Pistikopoulos (1995). First, they addressed the problem considering that the uncertainty profile is given. Therefore, the formulation is simplified to a single level DAE problem, with the objective of minimizing u for the flexibility test problem or maximizing δ for the flexibility index problem (where u and δ are scalar variables that account for the constraint violation and is related to the size of the uncertainty set, respectively). Then they addressed the general case where no specific knowledge about the uncertainty profile is assumed. The differential equations are converted into algebraic residual equations using orthogonal collocation on finite elements (Biegler 2010) and then ASM (Grossmann and Floudas 1987) is applied to the transformed model. The proposed methodology was applied to a simple system solved by Generalized Benders Decomposition (Geoffrion 1972).

Flexibility and stability together were first studied by Jiang *et al.* (2014). Based on existing algorithms for flexibility analysis, the vertex enumeration and the active set method (ASM), the authors extend the analysis to incorporate stability constraints. In the vertex enumeration method, a constraint stating that all the real parts of the eigenvalues of the Jacobian matrix of the equality constraints must be smaller than zero is added. For the ASM, the stability of the obtained flexible region is checked iteratively by choosing a new set of active constraints whose real part is less than zero. In addition, these authors proposed a new formulation using eigenvalue optimization methods, where one of the major difficulties of the integration of flexibility and stability lies on how to convert the Lyapunov stability conditions into model constraints embedded in the optimization problem. The authors transformed the necessary condition of stability, where the real part of the eigenvalues must be smaller than zero into the positive definiteness of a real symmetric matrix to explicitly express the stability condition.

To overcome the corresponding computational expense, Chen *et al*. (2018) proposed to incorporate a stability constraint obtained by the application of the singularity theory based stability analysis method. First, the singularity points are identified, and then the dynamic trajectories of singularity points extracted from the series of curves are regressed into functions of uncertain parameters and control variables, which are embedded into the flexibility analysis formulation as model constraints.

Controllability, another operability consideration, was incorporated in the flexibility analysis by Bahri *et al*. (1997) and later by Escobar *et al.* (2013), in which the control strategy is explicitly considered at the operating stage by the use of controllability metrics in order to design a heat exchanger network.

Many efforts have been dedicated to study a variety of aspects related to the flexibility analysis during the last decades. For a more exhaustive review and a historical perspective on this topic, the interested reader is referred to Grossmann *et al.* (2014) and Zhang *et al.* (2016). However, most of these formulations are based on the assumption that during operation stage uncertain parameters can be measured with precision to take the corrective action. Ostrovsky *et al*. (2003) and Rooney and Biegler (2003) extended the flexibility analysis by grouping the uncertain parameters, $\theta \in T$, into two types, measured (θ_m) and unmeasured (θ_u) parameters. The flexibility constraint was then extended to account for model parameters, θ_u, that cannot be measured or whose estimation cannot be improved during the operating stage.

In this paper, we propose new reformulations of the extended flexibility analysis where the innermost problems are recursively replaced by their optimality conditions and the complementarity conditions are expressed with mixed-integer constraints. We present the problem statement and motivations in Section 2. Special cases are considered to simplify the solution of the extended flexibility test in Section 3, where an upper bound formulation is derived in section 3.4 and illustrative examples are presented in Sections 3.5 and 3.6. The MINLP formulation for the general case is derived in full detail in Section 4. In Section 5, an alternative formulation is presented also for the general case. After that, Section 6 extends the proposed formulations for the models with equality constraints. The formulations are applied to a variety of examples in Section 7 and finally conclusions are drawn.

2. Problem Statement and Methodology

The basic model for the flexibility analysis involves design variables, d, control variables, z, state variables, x, and uncertain parameters, θ. The physical performance of a chemical process can be described by the following set of constraints

$$h_i(d, z, x, \theta) = 0 \quad i \in I \tag{6}$$

$$g_j(d, z, x, \theta) \leq 0 \quad j \in J \tag{7}$$

where h_i are the equations $i \in I$ (e.g. mass and energy balances or equilibrium relations) which hold for steady-state operation of the process, and g_j are the inequalities $j \in J$ (e.g. design specifications or physical operating limits) which must be satisfied in order to obtain feasible operation.

Generally, the state variables x can be expressed as an implicit function of the design variables d, control variables z with parameters θ using the equalities h.

$$h(d, z, x, \theta) = 0 \implies x = x(d, z, \theta) \tag{8}$$

This allows the elimination of the state variables x, as the performance specifications of the process can be described by the set of reduced inequality constraints in (9).

$$g_j\big(d, z, x(d, z, \theta)\big) = f_j(d, z, \theta) \leq 0 \; j \in J \tag{9}$$

For the sake of convenience, in this paper we will focus on the reduced model. However, we will take into account extensions to equality constraint in Section 6. One of the main problems addressed in the flexibility analysis is the flexibility test problem. It consists in determining whether for a fixed design d by proper adjustment of the control variables z, the process constraints $f_j(d, z, \theta) \leq 0$, $j \in J$, hold for any realization of uncertain parameters θ (Halemane and Grossmann 1983). This statement can be expressed with the logic expression (1), and is reformulated by the use of min and max operators as shown in Eq. (2).

The flexibility test problem determines whether a design d does or does not meet the flexibility target. To determine how much flexibility can be achieved in a given design, the flexibility index is defined as the largest value of δ for the uncertainty set $T = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\}$ where θ^N are nominal values and $\Delta\theta^+$, $\Delta\theta^-$ are positive and negative expected deviation, and such that the model inequalities hold over the set T (Swaney and Grossmann 1985).

The main difference between the design and control variables is that the design variables d are fixed during the operation stage, while the control variables z can be adjusted in order to satisfy process constraints. This implicitly requires having an accurate estimation of the uncertain parameters θ, an assumption that is often not met in practice.

To address these limitations, two groups of uncertain parameters are identified. The first group of uncertain parameters contains parameters whose values can be determined within any desired accuracy at the operation stage, namely the measured uncertain parameters, θ_m. Meaning that appropriate sensors are available to determine accurate values of all the uncertain parameters by direct measurement or by solving parameter estimation problems. Therefore, recourse action can be taken in order to compensate for their variation. Examples of this type of parameters include process conditions such as feed flowrates, pressures, temperatures, concentrations, and input variables such as product demands and electricity prices. The second group includes the unmeasured uncertain parameters, θ_u, whose estimation cannot be performed or improved during the operation stage, and consequently no control actions can be applied to them.

This distinction was made by Ostrovsky *et al.* (2003) and Rooney and Biegler (2003), who extended the logic constraint and the flexibility constraint into Eqs. (10) and (11), respectively.

$$\forall\, \theta_m \in T_m \left\{\exists\, z\ (\forall\, \theta_u \in T_u, \forall\, j \in J\big[f_j(d, z, \theta_m, \theta_u) \leq 0\big])\right\} \tag{10}$$

$$\chi(d) = \max_{\theta_m \in T_m} \min_{z} \max_{\theta_u \in T_u} \max_{j \in J} f_j(d, z, \theta_m, \theta_u) \leq 0 \tag{11}$$

where $T_m = \{\theta_m | \theta_m^L \leq \theta_m \leq \theta_m^U\}$ and $T_u = \{\theta_u | \theta_u^L \leq \theta_u \leq \theta_u^U\}$.

To solve the extended flexibility analysis, Ostrosvky *et al.* (2003) suggested an algorithm for calculation of the flexibility function based on a branch and bound strategy, while partitioning the uncertain set into subregions. On the other hand, Rooney and Biegler (2003) proposed an extension to the approach presented by Raspanti *et al.* (2000), which involves the use of the KS smooth function (Kreisselmeier and Steinhauser 1983) that aggregates all of the model inequality constraints, and the KKT derivation together with a smooth approximation of the complementarity conditions for the inner optimization problems. Therefore, the extended flexibility constraint results in a nonlinear programming program. It is worth noting that the innermost optimization problem is directly replaced by the smooth KS approximation. However, the linearity, if present, cannot be preserved, and even if the original constraints are convex, the resulting problem is non-convex (maximization of a convex objective function), which may lead to local solutions. Another drawback of the use of smoothing functions is that they can lead to ill-conditioned problems.

In this work, we reformulate the extended flexibility constraint by developing the KKT optimality conditions for each nested problem. In addition, in order to make the formulation tighter, the bounds of the nonnegative Lagrange multipliers related to the inequality constraints and the bounds on the slack variables are treated as model constraints of the following level optimization problem. Finally, we express the complementarity conditions with a mixed-integer representation and assume that the Haar condition holds, which states that the number of active constraints is equal to the dimension of the control variables plus one. This condition holds true provided the Jacobian is full rank (Grossmann and Floudas 1987).

In the following subsections, we derive the formulations of different cases: convex constraints, constraints with monotonic variation of both type of uncertain parameters and of unmeasured parameters with respect to model constraints, two formulations for general nonlinear constraints, and extensions to equality constraints.

3. Special Cases

In this section, we consider a special type of models where the multi-level problem can be simplified. In the following subsections, we will consider models characterized by convex functions, nonlinear functions with a monotonic variation with respect to both type uncertain parameters and with respect to unmeasured uncertain parameters only.

First, we make use of following property of multilevel problems (McKinsey 1952):

$$\max_x \max_y f(x,y) \leftrightarrow \max_y \max_x f(x,y) \tag{12}$$

as the order of the inner max operators is interchangeable and Eq. (11) can be equivalently expressed as follows:

$$(P1): \qquad \chi(d) = \max_{\theta_m \in T_m} \psi(d,\theta_m)$$

$$s.t.\ \psi(d,\theta_m) = \min_{z,u} \zeta(d,z,\theta_m)$$

$$s.t\ \zeta(d,z,\theta_m) = \max_{j\in J} \max_{\theta_u \in T_u} f_j(d,z,\theta_m,\theta_u)$$

where $T_m = \{\theta_m | \theta_m^L \le \theta_m \le \theta_m^U\}$ and $T_u = \{\theta_u | \theta_u^L \le \theta_u \le \theta_u^U\}$.

3.1. Extended Flexibility Test for Convex Constraints

If the constraint functions $f_j(d,z,\theta_m,\theta_u)$ are jointly 1-D quasi-convex in z, θ_m and θ_u, then the solution θ_u^* must lie at a vertex of T_u. Then $\zeta(d,z,\theta_m) = \max_{\theta_u \in T_u} f_j(d,z,\theta_m,\theta_u^*)$ is still a convex in z and θ_m. Therefore, $\psi(d, \theta_m) = \min_{z,u} \zeta(d, z, \theta_m)$ is a convex problem, this implies that $\psi(d, \theta_m)$ is also convex, thus $\psi(d, \theta_m) \leq 0$ defines a convex region in θ_m and implies that θ_m^* is also a vertex solution.

Then, the solution can be obtained by vertex enumeration:

$$\psi(d, \theta_m^v) = \min_{z,u} u^v$$
$$s.t. f_j(d, z, \theta_m^v, \theta_u^v) \leq u^v \ \forall \in J \tag{13}$$

where u^v is a scalar variable that represents the worst constraint violation at vertex v and V is the set of all 2^{np} vertices of T_m and T_u. A negative value of u implies that feasible operation can be ensured over the whole range of variation of the uncertain parameters for a fixed design d, otherwise it cannot be ensured. Then solution corresponds to the largest value of u^v obtained among the 2^{np} vertices in V.

$$\chi(d) = \max_{v \in V}\{ \psi(d, \theta_m^v)\} \tag{14}$$

3.2. Extended Flexibility Test for Constraints with Monotonic Variation of Unmeasured and Measured Uncertain Parameters

In this section, we consider that the innermost problem of *(P1)* is described by monotonic functions with respect to θ_u and θ_m.

Definition

Let f be defined on a set S. We say that f increases on the set S if and only if, for each $x \in S$ and $y \in S$ with $x < y$, then $f(x) \leq f(y)$. If strict inequality always holds, f is strictly increasing on the set S. An analogous definition hold for decreasing and strictly decreasing. A function that is either increasing or decreasing is called monotone.

An important feature of this type of functions is that their derivative is one-signed, i.e. $\partial f_j / \partial \theta_u \ \forall \ j \in J$ and $\partial f_j / \partial \theta_m \ \forall \ j \in J$ are one-singed.

Theorem 1

(i)Without loss of generality, suppose that f is increasing and bounded above on (a, b) with smallest upper bound U. Then $f(x) \to U$ as $x \to b^-$.

(ii) Let f be increasing and bounded below on (a, b) with largest lower bound L. Then $f(x) \to L$ as $x \to a^+$.

Proof (Binmore 1982).

(i) For any $\epsilon > 0$, there is a δ such that $b - \delta < x < b \Rightarrow |f(x) - U| < \epsilon$.
i.e. $U - \epsilon < f(x) < U + \epsilon$

The inequality $f(x) < L + \epsilon$ is automatically satisfied because $U$is an upper bound for f on (a, b). Since $U - \epsilon$ is not an upper bound for f on (a, b), there exists a $c \in (a, b)$ such that $U - \epsilon < f(c)$. But f increases on (a, b), therefore for any x satisfying $c < x < b$, then $U - \epsilon < f(c) \leq f(x)$, where $\delta = b - c$. □

Hence, the solution θ_u^* and θ_m^* of problem *(P1)* must lie in one of the extreme points T_u and T_m, respectively. It can be obtained solving problem (13) for each vertex in V to global optimality and then computing the worst constraint violation with (14).

3.3. Extended Flexibility Test for Constraints with Monotonic Variation of Unmeasured Uncertain Parameters

If the innermost problem of *(P1)* is described by monotonic functions with respect to θ_u, its solution for can be computed by performing the traditional flexibility test for the measured uncertain parameters with a vertex enumeration of the unmeasured uncertain parameters. The bilevel problems *(P2)* described are obtained by fixing the unmeasured uncertain parameters to the value of each vertex point.

$$(P2):\ \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m)$$

$$s.t.\ \ \psi(d, \theta_m) = \min_{z,u} u$$

$$s.t.\ f_j(d, z, \theta_m, \theta_u^v) \leq u, \forall\, j \in J$$

The inequalities f_j are expressed as equality constraints by the introduction of nonnegative slack variables, s_j^0. The Lagrangean function of the lower level problem, $\psi(d, \theta_m)$, is then described by Eq. (15), which is a parametrization of the design variables, d, and the measured uncertain parameters, θ_m.

$$\mathcal{L}_0(d, \theta_m) = u + \sum_j \lambda_j^0 \cdot \left(f_j(d, z, \theta_m, \theta_u^v) - u + s_j^0\right) \tag{15}$$

We apply the active set strategy (Grossmann and Floudas 1987) to obtain a single level optimization problem for each vertex v. In other words, the lower level problem of *(P2)* is replaced by its KKT conditions (Eqs. (16) to (18)) and complementarity conditions (Eq. (19)).

$$\frac{\partial \mathcal{L}_0}{\partial u} = 1 - \sum_j \lambda_j^0 = 0 \tag{16}$$

$$\frac{\partial \mathcal{L}_0}{\partial z} = \sum_j \lambda_j^0 \cdot \frac{\partial f_j}{\partial z} = 0 \tag{17}$$

$$\frac{\partial \mathcal{L}_0}{\partial \lambda_j^0} = f_j(d, z, \theta_m, \theta_u^v) - u + s_j^0 = 0, \;\; \forall \;\; j \in J \tag{18}$$

$$\lambda_j^0 \cdot s_j^0 = 0, \qquad \lambda_j^0, s_j^0 \;\geq 0, \;\; \forall \;\; j \in J \tag{19}$$

It should be noted that discrete decisions are involved in the complementarity conditions, since they define the selection of active set of constraints (Grossmann and Floudas 1987). They can be replaced by the following set of 0-1 mixed-integer constraints.

$$\lambda_j^0 - y_j^0 \leq 0, \qquad \forall \;\; j \in J \tag{20}$$

$$s_j^0 - M\left(1 - y_j^0\right) \leq 0, \qquad \forall \;\; j \in J \tag{21}$$

$$\lambda_j^0, s_j^0 \;\geq 0, \qquad y_j^0 \in \{0,1\}, \qquad \forall\, j \in J \tag{22}$$

where M represents an upper bound for the slacks. Necessary and complementarity conditions expressed with a mixed-integer representation are replaced in problem *(P2)* leading to v single level MILP/MINLP problem for every $v \in V$.

$$(P3): \qquad \chi^v(d) = \max_{\theta_m \in T_m} u^v \tag{23}$$

$$s.t. \;\; \theta_m^{LB} \leq \theta_m \leq \theta_m^{UB} \tag{24}$$

$$1 - \sum_j \lambda_j^0 = 0 \tag{25}$$

$$\sum_j \lambda_j^0 \cdot \frac{\partial f_j}{\partial z} = 0 \tag{26}$$

$$f_j(d, z, \theta_m, \theta_u^v) - u^v + s_j^0 = 0, \qquad \forall \ \ j \in J \tag{27}$$

$$\lambda_j^0 - y_j^0 \leq 0, \qquad\qquad \forall \ \ j \in J \tag{28}$$

$$s_j^0 - M\left(1 - y_j^0\right) \leq 0, \qquad \forall \ \ j \in J \tag{29}$$

$$\sum_j y_j^0 \leq n_z + 1 \tag{30}$$

$$\lambda_j^0, s_j^0 \ \geq 0, \qquad y_j^0 \in \{0,1\} \ \forall \, j \in J \tag{31}$$

In addition, Eq. (30) enforces the constraint that the potential sets of active constraints are at most $n_z + 1$, where n_z stands for the dimension of the vector of control variables z.

Take for example a system with two unmeasured uncertain parameters, where the unmeasuerd uncertain parameter set has four vertices. θ_u is fixed at the diferent vertices: and the traditional flexibility analysis is performed four times (one time for each vertex). The solution corresponds to the largest value of u^v obtained along the vertices.

$$\begin{gathered} \chi(d) = \max_{v \in V}\{\chi^v(d)\} \\ \chi^v(d) = \max_{\theta_m \in T_m} \min_{z,u}(u^v | f_j(d, z, \theta_m, \theta_u^v) \leq u^v, j \in J) \end{gathered} \tag{32}$$

where v are the vertices $\{\theta_{u_1}^{LB}, \theta_{u_2}^{LB}; \theta_{u_1}^{LB}, \theta_{u_2}^{UB}; \theta_{u_1}^{UB}, \theta_{u_2}^{LB}; \theta_{u_1}^{UB}, \theta_{u_2}^{UB}\}$ for the case of two unmeasured uncertain parameters, and u_v is computed by solving *(P3)* at each vertex of the unmeasured uncertain parameter set.

3.4. Upper Bound of Extended Flexibility Test

In order to avoid the vertex enumeration, an upper bound of the extended flexibility analysis can be computed. As already mentioned, the solution of the innermost problem

(P1) must lie in one of the extreme points of its range of variation. Then, the value of θ_u can be fixed for each constraint $j \in J$ depending on the sign of the derivative, $\partial f_j/\partial\theta_{u_j}$ as follows.

$$\frac{\partial f_j}{\partial\theta_{u_j}} \geq 0 \Rightarrow \theta_{u_j}^* = \theta_u^{UB} \tag{33}$$

$$\frac{\partial f_j}{\partial\theta_{u_j}} < 0 \Rightarrow \theta_{u_j}^* = \theta_u^{LB} \tag{34}$$

If the set of functions $f_j(d, z, \theta_m, \theta_u)$ varies monotonically with respect to the unmeasured uncertain parameters, then the relationship expressed by Eqs. (33) and (34) holds true and the bilevel problem *(P4)* is obtained by replacing Eqs. (33) and (34) in (P1).

$$(P4): \qquad \chi^{UB}(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m)$$

$$\textit{s.t.} \;\; \psi(d, \theta_m) = \min_{z,u} u$$

$$\textit{s.t.} \;\; f_j\left(d, z, \theta_m, \theta_{u_j}^*\right) \leq u, \;\; \forall \;\; j \in J$$

Similarly, *(P4)* is reformulated following the active set strategy (Grossmann and Floudas 1987) but in this case leading to only one MILP/MINLP problem.

$$(P5): \qquad \chi^{UB}(d) = \max_{\theta_m \in T_m} u$$

$$\textit{s.t.} \;\; \theta_m^{LB} \leq \theta_m \leq \theta_m^{UB}$$

$$1 - \sum_j \lambda_j^0 = 0$$

$$\sum_j \lambda_j^0 \cdot \frac{\partial f_j}{\partial z} = 0$$

$$f_j\left(d, z, \theta_m, \theta_{u_j}^*\right) - u + s_j^0 = 0, \qquad \forall \;\; j \in J$$

$$\lambda_j^0 - y_j^0 \leq 0, \qquad \forall \;\; j \in J$$

$$s_j^0 - M\left(1 - y_j^0\right) \leq 0, \qquad \forall \;\; j \in J$$

$$\sum_j y_j^0 \leq n_z + 1$$

$$\lambda_j^0, s_j^0 \;\geq 0, y_j^0 \in \{0,1\}, \qquad \forall \;\; j \in J$$

It is important to note that even though the solution lies at one of the vertices of the unmeasured uncertain parameter set for systems with monotonic variation of the unmeasured uncertain parameters, fixing the values of θ_u at different extreme points simultaneously leads to an upper bound of the solution.

3.5. Linear Example

In this section, we illustrate the extended flexibility analysis for a convex case. Consider the following linear example, described by three inequalities with a single control variable, z, and two uncertain parameters, θ_1 and θ_2.

$$f_1 = z - \theta_1 + 2 \cdot \theta_2 - 5 \leq 0 \tag{35}$$

$$f_2 = -z - \frac{\theta_1}{3} - \frac{\theta_2}{2} - 3 \leq 0 \tag{36}$$

$$f_3 = z + \theta_1 - \theta_2 - 6 \leq 0 \tag{37}$$

We calculate the flexibility test of the inequalities to over the specified uncertain set $0 \leq \theta_1 \leq 8$, $0 \leq \theta_2 \leq 5$. As there is one control variable, there are two active constraints at the solution. We identify two sets of active constraints: active set 1 involves constraints f_1 and f_2, and active set 2 involves f_2 and f_3. Then, we project the feasible region into the space of $\theta \cdot u$ by taking into account the potential active sets.

First, we consider the case that control actions can compensate for all the uncertain parameters, therefore we apply the active set method formulation of the traditional flexibility analysis described by problem (PA1) to solve the flexibility test problem. In

Figure 1, we present the projection of the feasible region onto the space $\theta \cdot u$, where the maximum value of u corresponds to point (i), which is a negative value (-0.25), implying that feasible operation can be ensured over the entire range of variation of the uncertain parameters. Numerical results of this case are detailed in the first column of Table 1.

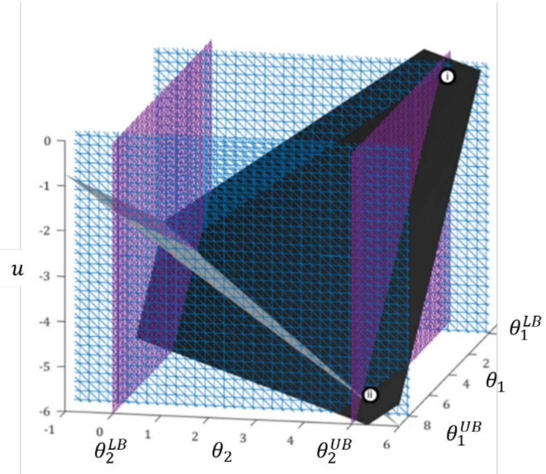


Figure 1. Projection of example 1 onto the space of the $\theta \cdot u$. (i) Maximum constraint violation, (ii) minimum constraint violation, black hyperplane: active set 1: f_1 and f_2, grey hyperplane: active set 2: f_2 and f_3.

Then, we consider the case that θ_1 corresponds to a measured uncertain parameter and θ_2 corresponds to an unmeasured uncertain parameter. Due to convexity, the solution of this system lies at one vertex of the uncertainty set, as previously explained in Section 3.1. Therefore, we solve Eq. (13) for each vertex. The corresponding results are presented in the second column of Table 1, where the worst constraint violation corresponds to -0.25, in agreement with the results obtained with the MILP of the active set method.

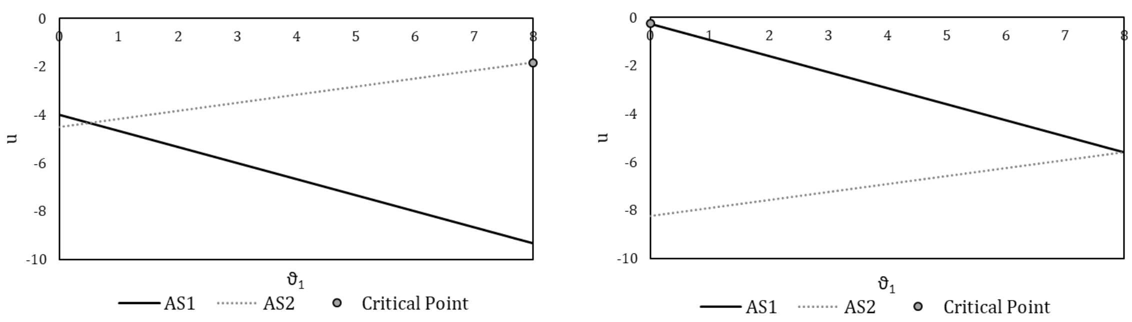
Table 1. Numerical results of the flexibility test for Linear Example.

	Traditional Flexibility Analysis $\theta_m = \{\theta_1, \theta_2\}$		*Extended Flexibility Analysis*	
	Active Set Method	*Vertex Enumeration* $\theta_m^{fixed} = \{\theta_1, \theta_2\}$	*Vertex Enumeration*	*Upper Bound*
			$\theta_m = \{\theta_1\}, \theta_u^{fixed} = \{\theta_2\}$	

u	**-0.25**	-4	-1.83	**-0.25**	-5.58	-1.83	**-0.25**	1
θ_1	0	θ_1^{LB}	θ_1^{UB}	θ_1^{LB}	θ_1^{UB}	8	0	0
θ_2	5	θ_2^{LB}	θ_2^{LB}	θ_2^{UB}	θ_2^{UB}	θ_2^{LB}	θ_2^{UB}	$\theta_{2_{j=1}} = \theta_2^{UB}$ $\theta_{2_{j=2}} = \theta_2^{UB}$ $\theta_{2_{j=3}} = \theta_2^{LB}$
y_1	1	A	I	A	I	0	1	1
y_2	1	A	A	A	A	1	1	1
y_3	0	I	A	I	A	1	0	0
z	-5.25	1	-3.83	-5.25	-2.58	-3.83	-5.25	-4
	MILP	LP				MILP		

Big M value: 500, solver: CPLEX, solver tolerance: 1E-6, A: active, I: inactive.

For the sake of comparison, we perform a vertex enumeration for the unmeasured uncertain parameter (θ_2). In other words, we solve *(P3)* fixing θ_u either to its lower or upper bound. Figure 2 shows the projection of the feasible region onto the space of $\theta_1 \cdot u$ for the two extreme values of θ_2. The result of the worst constraint violation (u=-0.25) is obtained when fixing the value of θ_2 to its upper bound as shown in Figure 2 (b), whereas when θ_2 is fixed at its lower bound the value of u corresponds to -1.83 (Figure 2 (a)). Therefore, the extended flexibility test is passed as the worst constraint violation is a negative value.



(a) (b)

Figure 2. Projection of feasible operation onto the space of the $\theta_1 \cdot u$ with θ_2 fixed at its (a) lower bound and (b) upper bound.

Finally, we calculate the upper bound of the extended flexibility test problem applying the formulation described by *(P5)*, where the values of θ_{2_j} are fixed depending on the sign of the derivative. We can see that we obtain a conservative solution (u=1), as the unmeasured uncertain parameter is set to two different values simultaneously.

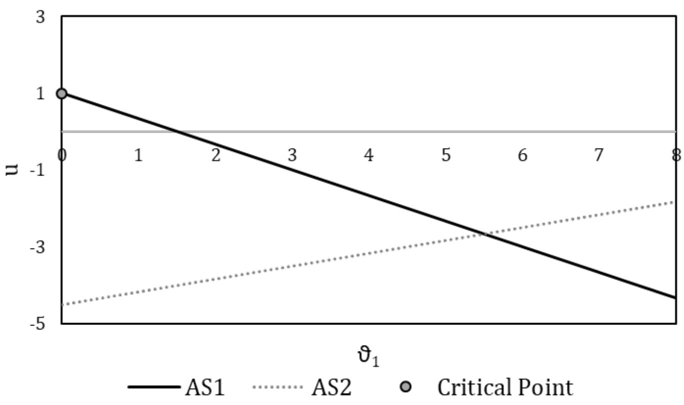


Figure 3. Projection of feasible operation onto the space of the $\theta_1 \cdot u$ with θ_{2_j} fixed depending on the sign of the derivative of function f_j with respect to θ_2.

It is important to note, that for convex problems the formulation can be simplified because the solution corresponds to a vertex solution.

3.6. Nonlinear Example

We perform a similar analysis as in the previous section. The example has been modified in order to account for nonlinear terms with monotonic variation with respect to both θ_1 and θ_2, such as cubic, arctangent and exponential functions.

$$f_1 = z - \theta_1^3 + 2 \cdot \theta_2 - 5 \leq 0 \tag{38}$$

$$f_2 = -z - \frac{\theta_1}{3} - \arctan(\theta_2) - 3 \leq 0 \tag{39}$$

$$f_3 = z + \theta_1 - \frac{1}{2^{\theta_2} + 1} - 6 \leq 0 \tag{40}$$

The flexibility test of the inequalities is performed over the same specified uncertain set $0 \leq \theta_1 \leq 8$, $0 \leq \theta_2 \leq 5$. First, we apply the active set method, formulation (PA1), to solve the flexibility test problem. Again, we show the projection of the feasible region onto the space $\theta \cdot u$ in Figure 4, where the maximum value of u =0.313 corresponds to point (i). In this case, feasible operation cannot be ensured over the entire range of variation of the uncertain parameters. The results are summarized in the first column of Table 2.

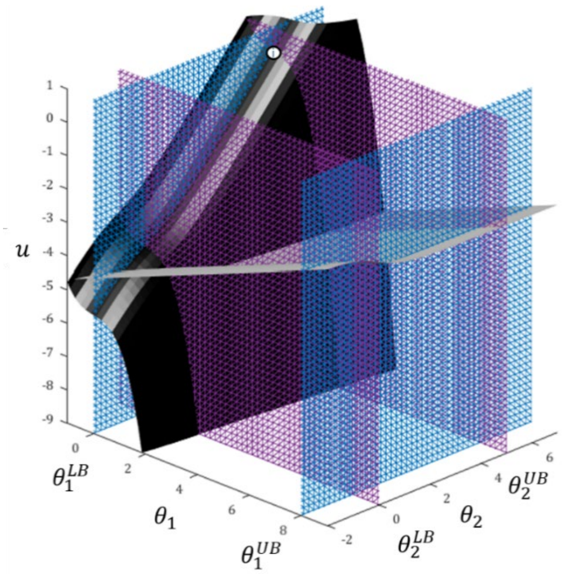


Figure 4. Projection of example 2 onto the space of the $\theta \cdot u$. (i) Maximum constraint violation, black hyperplane: active set 1: f_1 and f_2, grey hyperplane: active set 2: f_2 and f_3.

The solution of this model also lies at one vertex of the uncertainty set, as explained in Section 3.2. Hence, we again solve Eq. (13) for each vertex. Numerical results are shown in the second column of Table 1. The maximum constraint violation is 0.313, this result is also in agreement with the results obtained with the active set method.

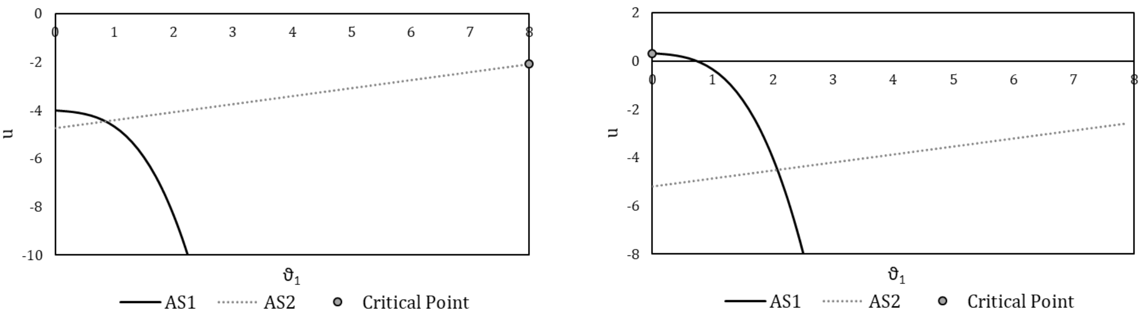
Table 2. Numerical results of the flexibility test for Nonlinear Example.

	Traditional Flexibility Analysis $\theta_m = \{\theta_1, \theta_2\}$					*Extended Flexibility Analysis*		
	Active Set Method	*Vertex Enumeration* $\theta_m^{fixed} = \{\theta_1, \theta_2\}$				*Vertex Enumeration*		*Upper Bound*
						$\theta_m = \{\theta_1\}, \theta_u^{fixed} = \{\theta_2\}$		
u	**0.313**	-4	-2.1	**0.313**	-2.54	-2.12	**0.313**	1
θ_1	0	θ_1^{LB}	θ_1^{UB}	θ_1^{LB}	θ_1^{UB}	8	0	0
θ_2	5	θ_2^{LB}	θ_2^{LB}	θ_2^{UB}	θ_2^{UB}	θ_2^{LB}	θ_2^{UB}	$\theta_{2_{j=1}} = \theta_2^{UB}$ $\theta_{2_{j=2}} = \theta_2^{UB}$ $\theta_{2_{j=3}} = \theta_2^{LB}$
y_1	1	A	I	A	I	0	1	1
y_2	1	A	A	A	A	1	1	1
y_3	0	I	A	I	A	1	0	0
z	-4.69	1	-3.58	-4.69	-4.51	-3.52	-4.69	-4
	MINLP	NLP				MINLP		

Big M value: 500, solver: LINDOGLOBAL, solver tolerance: 1E-6. A: active, I: inactive.

Additionally, we apply the extended flexibility test considering θ_1 as a measured uncertain parameter and θ_2 as an unmeasured uncertain parameter by performing a vertex enumeration for the unmeasured uncertain parameter, where problem (*P3*) is solved at each vertex of T_u.

In Figure 5, we present the projection of the feasible region onto the space of $\theta_1 \cdot u$ for the two extreme values of θ_2. The result of the worst constraint violation (u=0.313) is obtained when fixing the value of θ_2 to its upper bound as shown in Figure 5 (b), whereas when θ_2 is fixed at its lower bound the value of u corresponds to -2.12 (Figure 5 (a)). In this case, the extended flexibility test is not passed, as the worst constraint violation is a positive value (0.313).



(a) (b)

Figure 5. Projection of feasible operation onto the space of the $\theta_1 \cdot u$ with θ_2 fixed at its (a) lower bound and (b) upper bound.

Moreover, we calculate the upper bound of the extended flexibility test problem by solving problem *(P5)*, where the values of θ_{2_j} are fixed depending on the sign of the derivative. We can see that again we obtain a conservative solution (u=1), as the unmeasured uncertain parameter is set to two different values simultaneously. The details of this case are summarized in the last column of Table 2.

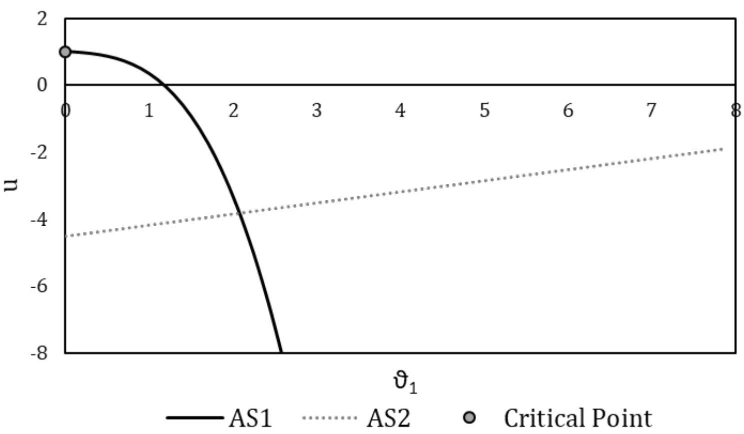


Figure 6. Projection of feasible operation onto the space of the $\theta_1 \cdot u$ with θ_{2_j} fixed depending on the sign of the derivative of function f_j with respect to θ_2.

4. General Case: NLP Problem

In this section, we present the reformulation for the general case of nonlinear model constraints. The extended flexibility constraint Eq. (11) can be equivalently expressed as the following multi-level optimization problem *(P6)*.

$$(P6): \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m) \tag{41}$$

$$s.t.\ \psi(d, \theta_m) = \min_z \zeta(d, z, \theta_m) \tag{42}$$

$$s.t.\ \zeta(d, z, \theta_m) = \max_{\theta_u \in T_u} \phi(d, z, \theta_m, \theta_u) \tag{43}$$

$$s.t.\ \phi(d, z, \theta_m, \theta_u) = \min_u u \tag{44}$$

$$s.t.\ f_j(d, z, \theta_m, \theta_u) \leq u, \quad \forall j \in J \tag{45}$$

In order to solve problem *(P6)*, we propose to replace the inner problems by their optimality conditions in a recursive fashion. Bounds of the nonnegative Lagrange multipliers and slack variables related to the inequality constraints are added as model constraints of the next level optimization problem in order to tighten the formulation. Following this procedure, we obtain a single level optimization problem. The complementarity conditions are represented with mixed-integer constraints, and the Haar conditions is assumed leading to an MINLP problem.

First, we consider the innermost minimization problem (Eqs. (44) and (45)). The Lagrangean function of this problem corresponds to Eq. (46), whose necessary conditions are described by Eqs. (47) and (48), and complementarity conditions by Eq. (49).

$$\mathcal{L}_0(d, z, \theta_m, \theta_u) = u + \sum_j \lambda_j^0 \cdot (f_j(d, z, \theta_m, \theta_u) - u + s_j^0) \tag{46}$$

$$\frac{\partial \mathcal{L}_0}{\partial \lambda_j^0} = f_j(d, z, \theta_m, \theta_u) - u + s_j^0 = 0, \qquad \forall\ j \in J \tag{47}$$

$$\frac{\partial \mathcal{L}_0}{\partial u} = 1 - \sum_j \lambda_j^0 = 0 \tag{48}$$

$$\lambda_j^0 \cdot s_j^0 = 0, \qquad \lambda_j^0, s_j^0 \ \geq 0, \qquad \forall \ j \in J \tag{49}$$

Then, the obtained expressions are replaced in *(P6)*, leading to a tri-level optimization problem *(P7)*. As already mentioned, the bounds of the nonnegative Lagrange multipliers and slack variables are added as model constraints. In addition, the bounds of the unmeasured uncertain parameters are also considered as model constraints. For the sake of simplicity, we consider the hyperrectangle set T_u to describe their variation.

$$\begin{aligned}
(P7)\colon \chi(d) = \max_{\theta_m \in T_m} \ & \psi(d, \theta_m) \\
s.t.\ \psi(d, \theta_m) = \min_z \ & \zeta(d, z, \theta_m) \\
& s.t.\ \zeta(d, z, \theta_m) = \max_{\theta_u \in T_u} \phi(d, z, \theta_m, \theta_u) \\
& \qquad s.t.\ (47) \text{ to } (49) \\
& \qquad \theta_{u_k}^{LB} - \theta_{u_k} \leq 0 \\
& \qquad \theta_{u_k} - \theta_{u_k}^{UB} \leq 0
\end{aligned}$$

After the first reformulation, the innermost problem corresponds to $\zeta(d, z, \theta_m)$, whose Lagrangean function is given as follows.

$$\begin{aligned}
\mathcal{L}_1(d, z, \theta_m) = & -u + \sum_j \mu_{1_j}^1 \cdot \left(f_j(d, z, \theta_m, \theta_u) - u + s_j^0 \right) + \sum_j \mu_{2_j}^1 \cdot (\lambda_j^0 \cdot s_j^0) \\
& + \mu_3^1 \cdot \left(1 - \sum_j \lambda_j^0 \right) + \sum_j \lambda_{1_j}^1 \cdot \left(-\lambda_j^0 + s_{1_j}^1 \right) + \sum_j \lambda_{2_j}^1 \cdot \left(-s_j^0 + s_{2_j}^1 \right) \\
& + \sum_k \lambda_{3_k}^1 \cdot \left(\theta_{u_k}^{LB} - \theta_{u_k} + s_{3_k}^1 \right) + \sum_k \lambda_{4_k}^1 \cdot \left(\theta_{u_k} - \theta_{u_k}^{UB} + s_{4_k}^1 \right)
\end{aligned} \tag{50}$$

The same procedure is applied to *(P7)* to obtain the bilevel problem *(P8)*. We first take the derivatives of the Lagrangean function ($\mathcal{L}_1$) with respect to the multipliers of the current level $\mu_{1_j}^1$, $\mu_{2_j}^1$, μ_3^1, $\lambda_{1_j}^1$, $\lambda_{2_j}^1$, $\lambda_{3_k}^1$, and $\lambda_{4_k}^1$ leading to equations (51) to (57), which correspond to innermost problem of *(P7)*.

$$\frac{\partial \mathcal{L}_1}{\partial \mu_{1_j}^1} = \frac{\partial \mathcal{L}_0}{\partial \lambda_j^0} = f_j(d, z, \theta_m, \theta_u) - u + s_j^0 = 0, \qquad \forall\, j \in J \tag{51}$$

$$\frac{\partial \mathcal{L}_1}{\partial \mu_{2_j}^1} = \lambda_j^0 \cdot s_j^0 = 0, \qquad \forall \ j \in J \tag{52}$$

$$\frac{\partial \mathcal{L}_1}{\partial \mu_3^1} = \frac{\partial \mathcal{L}_0}{\partial u} = 1 - \sum_j \lambda_j^0 = 0 \tag{53}$$

$$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1_j}^1} = -\lambda_j^0 + s_{1_j}^1 = 0, \qquad \forall j \in J \tag{54}$$

$$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2_j}^1} = -s_j^0 \ + s_{2_j}^1 = 0, \qquad \forall j \in J \tag{55}$$

$$\frac{\partial \mathcal{L}_1}{\partial \lambda_{3_k}^1} = \theta_{u_k}^{LB} - \theta_{u_k} + s_{3_k}^1 \ = 0, \qquad \forall \ \ k \in K \tag{56}$$

$$\frac{\partial \mathcal{L}_1}{\partial \lambda_{4_k}^1} = \theta_{u_k} - \theta_{u_k}^{UB} + s_{4_k}^1 = 0, \qquad \forall \ \ k \in K \tag{57}$$

Then, we take the derivatives of the Lagrangean function with respect to the worst constraint violation variable, u, the unmeasured uncertain parameters, θ_{u_k}, slack variables, s_j^0, and nonnegative Lagrange multiplier of previous level, λ_j^0.

$$\frac{\partial \mathcal{L}_1}{\partial u} = -1 - \sum_j \mu_{1_j}^1 = 0 \tag{58}$$

$$\frac{\partial \mathcal{L}_1}{\partial \theta_{u_k}} = \sum_j \mu_{1_j}^1 \cdot \frac{\partial f_j}{\partial \theta_{u_k}} - \lambda_{3_k}^1 + \lambda_{4_k}^1 = 0, \qquad \forall \ \ k \in K \tag{59}$$

$$\frac{\partial \mathcal{L}_1}{\partial s_j^0} = \mu_{1_j}^1 + \mu_{2_j}^1 \cdot \lambda_j^0 - \lambda_{2_j}^1 = 0, \qquad \forall \ \ j \in J \tag{60}$$

$$\frac{\partial \mathcal{L}_1}{\partial \lambda_j^0} = \mu_{2_j}^1 \cdot s_j^0 - \mu_3^1 - \lambda_{1_j}^1 = 0, \qquad \forall \ \ j \in J \tag{61}$$

Finally, we include the complementarity conditions of the lower bounds of Lagrange multipliers and slack variables, and lower and upper bound of θ_{u_k}.

$$\lambda^1_{1_j} \cdot s^1_{1_j} = 0, \qquad \lambda^1_{1_j}, s^1_{1_j} \geq 0, \qquad \forall\, j \in J \tag{62}$$

$$\lambda^1_{2_j} \cdot s^1_{2_j} = 0, \qquad \lambda^1_{2_j}, s^1_{2_j} \geq 0, \qquad \forall\, j \in J \tag{63}$$

$$\lambda^1_{3_k} \cdot s^1_{3_k} = 0, \qquad \lambda^1_{3_k}, s^1_{3_k}, \geq 0\,, \qquad \forall\;\; k \in K \tag{64}$$

$$\lambda^1_{4_k} \cdot s^1_{4_k} = 0, \qquad \lambda^1_{4_k}, s^1_{4_k} \geq 0\,, \qquad \forall\;\; k \in K \tag{65}$$

We replace Eqs. (51) to (65) in *(P7*) in order to obtain the bilevel problem *(P8)*. In this level, the bounds of the control variables are also considered as model constraints.

$$
\begin{aligned}
(P8)\!: \ \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m) \\
s.t.\ \psi(d, \theta_m) = \min_{z} \zeta(d, z, \theta_m) \\
s.t.\ (51) \text{ to } (65) \\
z_n^{LB} - z_n \leq 0, \qquad \forall\;\; n \in N \\
z_n - z_n^{UB} \leq 0, \qquad \forall\;\; n \in N
\end{aligned}
$$

The Lagrangean function of *(P8)*, $\mathcal{L}_2$, is described by Eq. (66).

$$
\begin{aligned}
\mathcal{L}_2(d,\theta_m) = {} & u + \sum_j \mu^2_{1_j} \cdot \left(f_j(d,z,\theta_m,\theta_u) - u + s^0_j\right) + \sum_j \mu^2_{2_j} \cdot (\lambda^0_j \cdot s^0_j) + \mu^2_3 \left(1 - \sum_j \lambda^0_j\right) \\
& + \mu^2_4 \cdot \left(-1 - \sum_j \mu^1_{1_j}\right) + \sum_k \mu^2_{5_k} \cdot \left(\sum_j \mu^1_{1_j} \cdot \frac{\partial f_j}{\partial \theta_{u_k}}\right) + \sum_j \mu^2_{6_j} \cdot \left(\mu^1_{1_j} + \mu^1_{2_j} \cdot \lambda^0_j - \lambda^1_{2_j}\right) \\
& + \sum_j \mu^2_{7_j} \cdot \left(\mu^1_{2_j} \cdot s^0_j - \mu^1_3 - \lambda^1_{1_j}\right) + \sum_j \mu^2_{8_j} \cdot \left(-\lambda^0_j + s^1_{1_j}\right) + \sum_j \mu^2_{9_j} \cdot \left(-s^0_j + s^1_{2_j}\right) \\
& + \sum_j \mu^2_{10_j} \cdot \left(\lambda^1_{1_j} \cdot s^1_{1_j}\right) + \sum_j \mu^2_{11_j} \cdot \left(\lambda^1_{2_j} \cdot s^1_{2_j}\right) + \sum_k \mu^2_{12_k} \cdot \left(\theta^{LB}_{u_k} - \theta_{u_k} + s^1_{3_k}\right) \\
& + \sum_k \mu^2_{13_k} \cdot \left(\theta_{u_k} - \theta^{UB}_{u_k} + s^1_{4_k}\right) + \sum_k \mu^2_{14_k} \cdot \left(\lambda^1_{3_k} \cdot s^1_{3_k}\right) + \sum_k \mu^2_{15_k} \cdot \left(\lambda^1_{4_k} \cdot s^1_{4_k}\right) \\
& + \sum_j \lambda^2_{1_j} \cdot \left(-\lambda^1_{1_j} + s^2_{1_j}\right) + \sum_j \lambda^2_{2_j} \cdot \left(-\lambda^1_{2_j} + s^2_{2_j}\right) + \sum_j \lambda^2_{3_j} \cdot \left(-s^1_{1_j} + s^2_{3_j}\right) \\
& + \sum_j \lambda^2_{4_j} \cdot \left(-s^1_{2_j} + s^2_{4_j}\right) + \sum_k \lambda^2_{5_k} \cdot \left(-\lambda^1_{3_k} + s^2_{5_k}\right) + \sum_k \lambda^2_{6_k} \cdot \left(-s^1_{3_k} + s^2_{6_k}\right) \\
& + \sum_k \lambda^2_{7_k} \cdot \left(-\lambda^1_{4_k} + s^2_{7_k}\right) + \sum_k \lambda^2_{8_k} \cdot \left(-s^1_{4_k} + s^2_{8_k}\right) + \sum_n \lambda^2_{9_n} \cdot \left(z^{LB}_n - z_n + s^2_{9_n}\right) \\
& + \sum_n \lambda^2_{10_n} \cdot \left(z_n - z^{UB}_n + s^2_{10_n}\right)
\end{aligned} \tag{66}
$$

The procedure is applied one more time in order to obtain the general MINLP formulation. Again, we take the derivative of the Lagrangean function ($\mathcal{L}_2$) with respect to the multipliers of the current level $\mu_{1_j}^2$, $\mu_{2_j}^2$, μ_3^2, μ_4^2, $\mu_{5_k}^2$, $\mu_{6_j}^2$, $\mu_{7_j}^2$, $\mu_{8_j}^2$, $\mu_{9_j}^2$, $\mu_{10_j}^2$, $\mu_{11_j}^2$, $\mu_{12_k}^2$, $\mu_{13_k}^2$, $\mu_{14_k}^2$, $\mu_{15_k}^2$, $\lambda_{1_j}^2$, $\lambda_{2_j}^2$, $\lambda_{3_j}^2$, $\lambda_{4_j}^2$, $\lambda_{5_k}^2$, $\lambda_{6_k}^2$, $\lambda_{7_k}^2$, $\lambda_{8_k}^2$, $\lambda_{9_n}^2$, and $\lambda_{10_n}^2$ leading to Eqs. (67) to (91), which correspond to innermost problem of *(P8)*.

$$\frac{\partial \mathcal{L}^2}{\partial \mu_{1_j}^2} = \frac{\partial \mathcal{L}_1}{\partial \mu_{1_j}^1} = \frac{\partial \mathcal{L}_0}{\partial \lambda_j^0} = f_j(d, z, \theta_m, \theta_u) - u + s_j^0 = 0, \qquad \forall\, j \in J \tag{67}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{2_j}^2} = \frac{\partial \mathcal{L}_1}{\partial \mu_{2_j}^1} = \lambda_j^0 \cdot s_j^0 = 0, \qquad \forall\;\; j \in J \tag{68}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_3^2} = \frac{\partial \mathcal{L}_1}{\partial \mu_3^1} = \frac{\partial \mathcal{L}_0}{\partial u} = 1 - \sum_j \lambda_j^0 = 0 \tag{69}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_4^2} = \frac{\partial \mathcal{L}_1}{\partial u} = -1 - \sum_j \mu_{1_j}^1 = 0 \tag{70}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{5_k}^2} = \frac{\partial \mathcal{L}_1}{\partial \theta_{u_k}} = \sum_j \mu_{1,j}^1 \cdot \frac{\partial f_j}{\partial \theta_{u_k}} - \lambda_{3_k}^1 + \lambda_{4_k}^1 = 0 \;\; \forall\;\; k \in K \tag{71}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{6_j}^2} = \frac{\partial \mathcal{L}_1}{\partial s_j^0} = \mu_{1_j}^1 + \mu_{2_j}^1 \cdot \lambda_j^0 - \lambda_{2_j}^1 = 0, \qquad \forall\;\; j \in J \tag{72}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{7_j}^2} = \frac{\partial \mathcal{L}_1}{\partial \lambda_j^0} = \mu_{2_j}^1 \cdot s_j^0 - \mu_3^1 - \lambda_{1_j}^1 = 0, \qquad \forall\;\; j \in J \tag{73}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{8_j}^2} = \frac{\partial \mathcal{L}_1}{\partial \lambda_{1_j}^1} = -\lambda_{1_j}^0 + s_{1_j}^1 = 0, \qquad \forall\;\; j \in J \tag{74}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{9_j}^2} = \frac{\partial \mathcal{L}_1}{\partial \lambda_{2_j}^1} = -s_{1_j}^0 + s_{2_j}^1 = 0, \qquad \forall\;\; j \in J \tag{75}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{10_j}^2} = \lambda_{1_j}^1 \cdot s_{1_j}^1 = 0, \qquad \forall\;\; j \in J \tag{76}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{11_j}^2} = \lambda_{2_j}^1 \cdot s_{2_j}^1 = 0, \qquad \forall\;\; j \in J \tag{77}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{12_k}} = \frac{\partial \mathcal{L}_1}{\partial \lambda^1_{3_k}} = \theta^{LB}_{u_k} - \theta_{u_k} + s^1_{3_k} \ = 0, \qquad \forall \ \ k \in K \tag{78}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{13_k}} = \frac{\partial \mathcal{L}_1}{\partial \lambda^1_{4_k}} = \theta_{u_k} - \theta^{UB}_{u_k} + s^1_{4_k} = 0, \qquad \forall \ \ k \in K \tag{79}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{14_k}} = \lambda^1_{3_k} \cdot s^1_{3_k} = 0, \qquad \forall \ \ k \in K \tag{80}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{15_k}} = \lambda^1_{4_k} \cdot s^1_{4_k} = 0, \qquad \forall \ \ k \in K \tag{81}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{1_j}} = -\lambda^1_{1_j} + s^2_{1_j} = 0, \qquad \forall \ \ j \in J \tag{82}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{2_j}} = -\lambda^1_{2_j} + s^2_{2_j} = 0, \qquad \forall \ \ j \in J \tag{83}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{3_j}} = -s^1_{1_j} + s^2_{3_j} = 0, \qquad \forall \ \ j \in J \tag{84}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{4_j}} = -s^1_{2_j} + s^2_{4_j} = 0, \qquad \forall \ \ j \in J \tag{85}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{5_k}} = -\lambda^1_{3_k} + s^2_{5_k} = 0, \qquad \forall \ \ k \in K \tag{86}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{6_k}} = -\lambda^1_{4_k} + s^2_{6_k} = 0, \qquad \forall \ \ k \in K \tag{87}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{7_k}} = -s^1_{3_k} + s^2_{7_k} = 0, \qquad \forall \ \ k \in K \tag{88}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{8_k}} = -s^1_{4_k} + s^2_{8_k} = 0, \qquad \forall \ \ k \in K \tag{89}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{9_n}} = z^{LB}_n - z_n + \ s^2_{9_n} - u = 0, \qquad \forall \ \ n \in N \tag{90}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda_{10_n}^2} = z_n - z_n^{UB} + \ s_{10_n}^2 - u = 0, \qquad \forall \ \ n \in N \tag{91}$$

Next, we compute the derivative of the Lagrangean function $\mathcal{L}_2$ with respect to the worst constraint violation variable, u, the unmeasured uncertain parameters, θ_{u_k}, the control variables, z_n, slack variables, s_j^0, $s_{1_j}^1$, $s_{2_j}^1$, $s_{3_k}^1$, $s_{3_k}^1$, $s_{4_k}^1$, and nonnegative Lagrange multiplier of previous level, λ_j^0, $\mu_{1_j}^1$, $\mu_{2_j}^1$, μ_3^1, $\lambda_{1_j}^1$, $\lambda_{2_j}^1$, $\lambda_{3_k}^1$, $\lambda_{4_k}^1$.

$$\frac{\partial \mathcal{L}_2}{\partial u} = 1 - \sum_j \mu_{1_j}^2 \ - \sum_n (\lambda_{9_n}^2 + \lambda_{10_n}^2) = 0 \tag{92}$$

$$\frac{\partial \mathcal{L}_2}{\partial \theta_{u_k}} = \sum_j \mu_{1_j}^2 \cdot \frac{\partial f_j}{\partial \theta_{u_k}} + \sum_{k'} \mu_{5_{k'}}^2 \cdot \sum_j \mu_{1,j}^1 \cdot \frac{\partial^2 f_j}{\partial \theta_{u_k} \partial \theta_{u_{k'}}} - \mu_{12_k}^2 + \mu_{13_k}^2 = 0 \qquad \forall \ \ k \in K \tag{93}$$

$$\frac{\partial \mathcal{L}_2}{\partial z_n} = \sum_j \mu_{1_j}^2 \cdot \frac{\partial f_j}{\partial z_n} + \sum_k \mu_{5_k}^2 \cdot \sum_j \mu_{1_j}^1 \cdot \frac{\partial^2 f_j}{\partial z_n \, \partial \theta_{u_k}} - \lambda_{9_n}^2 + \lambda_{10_n}^2 = 0 \qquad \forall \ \ n \in N \tag{94}$$

$$\frac{\partial \mathcal{L}_2}{\partial s_j^0} = \mu_{1_j}^2 + \mu_{2_j}^2 \cdot \lambda_j^0 + \mu_{7_j}^2 \cdot \mu_{2_j}^1 - \mu_{9_j}^2 = 0, \qquad \forall \ \ j \in J \tag{95}$$

$$\frac{\partial \mathcal{L}_2}{\partial s_{1_j}^1} = \mu_{8_j}^2 + \ \mu_{10_j}^2 \cdot \lambda_{1_j}^1 - \lambda_{3_j}^2 = 0, \qquad \forall \ \ j \in J \tag{96}$$

$$\frac{\partial \mathcal{L}_2}{\partial s_{2_j}^1} = \mu_{9_j}^2 + \ \mu_{11_j}^2 \cdot \lambda_{2_j}^1 - \lambda_{4_j}^2 \ = 0 \, , \qquad \forall \ \ j \in J \tag{97}$$

$$\frac{\partial \mathcal{L}_2}{\partial s_{3_k}^1} = \mu_{12_k}^2 + \mu_{14_k}^2 \cdot \lambda_{3_k}^1 - \ \lambda_{6_k}^2 = 0, \qquad \forall \, k \in K \tag{98}$$

$$\frac{\partial \mathcal{L}_2}{\partial s_{4_k}^1} = \mu_{13_k}^2 + \mu_{15_k}^2 \cdot \lambda_{4_k}^1 - \ \lambda_{8_k}^2 = 0, \qquad \forall \, k \in K \tag{99}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda_j^0} = \mu_{2_j}^2 \cdot s_j^0 - \mu_3^2 + \mu_{6_j}^2 \cdot \mu_{2_j}^1 - \mu_{8_j}^2 = 0, \qquad \forall \, j \in J \tag{100}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{1_j}^1} = -\mu_4^2 + \sum_k \mu_5^2 \cdot \frac{\partial f_j}{\partial \theta_{u_k}} + \mu_{6_j}^2 = 0, \qquad \forall \, j \in J \tag{101}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_{2_j}^1} = \mu_{6_j}^2 \cdot \lambda_j^0 + \mu_{7_j}^2 \cdot s_j^0 = 0, \qquad \forall \;\; j \in J \tag{102}$$

$$\frac{\partial \mathcal{L}_2}{\partial \mu_3^1} = -\sum_j \mu_{7_j}^2 = 0 \tag{103}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda_{1_j}^1} = -\mu_{7_j}^2 + \mu_{10_j}^2 \cdot s_{1_j}^1 - \lambda_{1_j}^2 = 0, \qquad \forall \;\; j \in J \tag{104}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda_{2_j}^1} = -\mu_{6_j}^2 + \mu_{11_j}^2 \cdot s_{2_j}^1 - \lambda_{2_j}^2 = 0, \qquad \forall \;\; j \in J \tag{105}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda_{3_k}^1} = \mu_{14_k}^2 \cdot s_{3_k}^1 - \lambda_{5_k}^2 = 0, \qquad \forall \;\; k \in K \tag{106}$$

$$\frac{\partial \mathcal{L}_2}{\partial \lambda_{4_k}^1} = \mu_{15_k}^2 \cdot s_{4_k}^1 - \lambda_{7_k}^2 = 0, \qquad \forall \;\; k \in K \tag{107}$$

The complementarity conditions of the third level are related with the lower bound of the Lagrange multipliers and slack variables related to original model constraints (Eq. (108)), and to the lower and upper bound of the unmeasured uncertain parameters (Eq. (109)). In addition, there are complementarity conditions related to the lower and upper bounds of the control variables (Eq. (110)).

$$\lambda_{l_j}^2 \cdot s_{l_j}^2 = 0, \qquad \forall \;\; j \in J, \qquad l = \{1, \dots, 4\} \tag{108}$$

$$\lambda_{l_k}^2 \cdot s_{l_k}^2 = 0, \qquad \forall \;\; k \in K, \qquad l = \{5, \dots, 8\} \tag{109}$$

$$\lambda_{l_n}^2 \cdot s_{l_n}^2 = 0\,, \qquad \forall \;\; n \in N, \qquad l = \{9, 10\} \tag{110}$$

The complementarity conditions presented in (108) to (110) are all replaced by the following mixed-integer constraints which for the sake of conciseness are written in generic form.

$$\lambda - M \cdot y \leq 0 \tag{111}$$

$$s - M \cdot (1 - y) \leq 0 \tag{112}$$

$$\lambda, s \geq 0, \qquad y \in \{0,1\} \tag{113}$$

where M corresponds to the Big M value.

The active set strategy is based on a determination of the potential sets of active constraints from the stationarity conditions by using the Property 1 in Grossmann and Floudas (1987) and the complementarity conditions.

$$\sum_j y_j^0 \leq n_z + 1 \tag{114}$$

where y_j^0 are binary variables to model the choice of the active set of original model constraints. Finally, the MINLP for the general case of extended flexibility analysis corresponds to *(P9)*.

$$(P9): \qquad \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m)$$

s.t. (67) to (110)

$$\sum_j y_j^0 \leq n_z + 1$$

The MINLP in *(P9)* is generally nonconvex and requires the use of a global optimization algorithms.

5. Alternative Reformulation

In order to study the effect of changing the order in Eq. (11) of the two innermost maximization problems, we propose and compare a different reformulation. The alternative reformulation to Eq. (11) is based on the property introduced in Section 3, which states that the order of the innermost maximization problems is interchangeable. Then the extended flexibility constraint can be expressed as follows.

$$\chi(d) = \max_{\theta_m \in T_m} \min_z \max_{j \in J} \max_{\theta_u \in T_u} f_j(d, z, \theta_m, \theta_u) \tag{115}$$

which is equivalently expressed,

$$(P10): \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m)$$

$$s.t.\ \psi(d,\theta_m) = \min_{z,u} \zeta(d,z,\theta_m)$$

$$s.t.\ \zeta(d,z,\theta_m) = \max_{\theta_u \in T_u} u$$

$$s.t.\ f_j(d,z,\theta_m,\theta_u) \le u, \quad \forall\, j \in J$$

$$\theta_{u_k}^{LB} \le \theta_{u_k} \le \theta_{u_k}^{UB}$$

(P10) is a tri-level problem, therefore the replacement of the inner problems by their optimality conditions must be performed twice (instead of thrice). The bounds on the unmeasured uncertain parameters, on the control variables and on the non-negative Lagrange multipliers and slack variables are considered as model constraints. The resulting single level optimization problem is provided for the alternative reformulation in Table B1.

6. Extension to Equality Constraints

Until now, we have been considering models described by a set of reduced inequality constraints. In this section, we consider the case of model consisting of equality and inequality constraints.

For the special cases *(P3)* and *(P5)*, we should note that if the non-reduced models contain equality constraints that do not depend on the unmeasured uncertain parameters, the MILP/MINLP problems can be easily extended to handle such a case. In case the unmeasured uncertain parameters are involved in the equality constraints, a monotonicity analysis must be performed in order to determine whether the formulations can be applied or not, and to determine the unmeasured uncertain parameters values in the upper bound reformulation. If the monotonicity analysis cannot be performed, the problem should be tackled with the general formulations.

For the general NLP problem, we follow a similar procedure as detailed in section 4 in order to obtain the single level optimization model. For the sake of completeness, we present the extended version of the alternative formulation in Table 3 and the extended version of the original formulation is provided in the Table C 1 of the Appendix C.

Table 3. Alternative formulation of a model consisting of equality and inequality constraints.

Description		*Equations*
Objective function		$(P11): \chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m)$
Model equality constraints	$\frac{\partial \mathcal{L}_1}{\partial \mu^1_{0_i}} = \frac{\partial \mathcal{L}_0}{\partial \mu^0_i}$	$h_i(d, z, \theta_m, \theta_u) = 0, \qquad \forall\ i\ \in I$
Model inequality constraints	$\frac{\partial \mathcal{L}_1}{\partial \mu^1_{1_j}} = \frac{\partial \mathcal{L}_0}{\partial \lambda^0_j} =$	$g_j(d, z, \theta_m, \theta_u) - u + s^0_j = 0, \forall\ \ j \in J$
1st level complementarity conditions	Original model constraints	$\lambda^0_j \cdot s^0_j = 0, \forall\ \ j \in J$
	Lower bound θ_u	$\lambda^0_{L_k} \cdot s^0_{L_k} = 0, \forall\ \ k \in K$
	Upper bound θ_u	$\lambda^0_{U_k} \cdot s^0_{U_k} = 0, \forall\ \ k \in K$
Derivatives w.r.t. model variables	$\frac{\partial \mathcal{L}_1}{\partial \mu^1_{5_k}} = \frac{\partial \mathcal{L}_0}{\partial \theta_{u_k}} =$	$\sum_{\boldsymbol{i}} \boldsymbol{\mu^0_i} \frac{\boldsymbol{\partial h_i}}{\boldsymbol{\partial \theta_{u_k}}} + \sum_j \lambda^0_j \frac{\partial g_j}{\partial \theta_{u_k}} - \lambda^0_{L_k} + \lambda^0_{U_k} = 0 \quad \forall\ \ k \in K$
Lower bound θ_u	$\frac{\partial \mathcal{L}_1}{\partial \mu^1_{6_k}} =$	$\theta^{LB}_{u_k} - \theta_{u_k} + s^0_{L_k} = 0,\ \ k \in K$
Upper bound θ_u	$\frac{\partial \mathcal{L}_1}{\partial \mu^1_{7_k}} =$	$\theta_{u_k} - \theta^{UB}_{u_k} + s^0_{U_k} = 0,\ \ k \in K$
Derivatives w.r.t. model variables	$\frac{\partial \mathcal{L}_1}{\partial u} =$	$1 - \sum_j \mu^1_{1_j} - \sum_n (\lambda^1_{L_n} + \lambda^1_{U_n}) = 0$
	$\frac{\partial \mathcal{L}_1}{\partial z_n} =$	$\sum_k \mu^1_{5_k} \cdot \left(\sum_{\boldsymbol{i}} \boldsymbol{\mu^0_i} \cdot \frac{\boldsymbol{\partial^2 h_i}}{\boldsymbol{\partial z_n \partial \theta_{u_k}}} + \sum_j \lambda^0_j \frac{\partial^2 g_j}{\partial z_n \partial \theta_{u_k}} \right) + \sum_{\boldsymbol{i}} \boldsymbol{\mu^1_{0_i}} \cdot \frac{\boldsymbol{\partial h_i}}{\boldsymbol{\partial z_n}} + \sum_j \mu^1_{1_j} \cdot \frac{\partial g_j}{\partial z_n} - \lambda^1_{L_n} + \lambda^1_{U_n} = 0 \quad \forall\ \ n \in N$
	$\frac{\partial \mathcal{L}_1}{\partial \theta_{u_k}} =$	$\sum_{k'} \mu^1_{5_{k'}} \cdot \left(\sum_{\boldsymbol{i}} \boldsymbol{\mu^0_i} \cdot \frac{\boldsymbol{\partial^2 h_i}}{\boldsymbol{\partial \theta_{u_k} \partial \theta_{u_{k'}}}} + \sum_j \lambda^0_j \frac{\partial^2 g_j}{\partial \theta_{u_k} \partial \theta_{u_{k'}}} \right) + \sum_{\boldsymbol{i}} \boldsymbol{\mu^1_{0_i}} \cdot \frac{\boldsymbol{\partial h_i}}{\boldsymbol{\partial \theta_{u_k}}} + \sum_j \mu^1_{1_j} \cdot \frac{\partial g_j}{\partial \theta_{u_k}} - \mu^1_{6_k} + \mu^1_{7_k} = 0 \quad \forall\ \ k \in K$
Derivatives w.r.t. slack variable	$\frac{\partial \mathcal{L}_1}{\partial s^0_j} =$	$\mu^1_{1_j} + \mu^1_{2_j} \cdot \lambda^0_j - \lambda^1_{2_j} = 0, \forall\ \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial s^0_{L_k}} =$	$\mu^1_{4_k} \cdot \lambda^0_{L_k} + \mu^1_{6_k} - \lambda^1_{2L_k} = 0, \forall\ \ k \in K$

Description		*Equations*
	$\frac{\partial \mathcal{L}_1}{\partial s_{U_k}^0} =$	$\mu_{3_k}^1 \cdot \lambda_{U_k}^0 + \mu_{7_k}^1 - \lambda_{2U_k}^1 = 0, \forall \ \ k \in K$
Derivatives w.r.t. Lagrange multiplier of previous level	$\frac{\partial \mathcal{L}_1}{\partial \mu_i^0} =$	$\boldsymbol{\sum_k \mu_{5_k}^1 \cdot \frac{\partial h_i}{\partial \theta_{u_k}} = 0}, \qquad \forall\ \boldsymbol{i \in I}$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_j^0} =$	$\mu_{2_j}^1 \cdot s_j^0 + \sum_k \mu_{5_k}^1 \frac{\partial g_j}{\partial \theta_{u_k}} - \lambda_{1_j}^1 = 0, \forall \ \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{L_k}^0} =$	$\mu_{4_k}^1 \cdot s_{L_k}^0 - \mu_{5_k}^1 - \lambda_{1L_k}^1 = 0, \forall \ \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{U_k}^0} =$	$\mu_{3_k}^1 \cdot s_{U_k}^0 + \mu_{5_k}^1 - \lambda_{1U_k}^1 = 0, \forall \ \ k \in K$
Lower bound z_n	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{L_n}^1} =$	$-z_n + z_n^{LB} + s_{L_n}^1 - u = 0, \forall \ \ n \in N$
Upper bound z_n	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{U_n}^1} =$	$z_n - z_n^{UB} + s_{U_n}^1 - u = 0, \forall \ \ n \in N$
Bounds on Lagrange multipliers and slack variables	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1_j}^1} =$	$-\lambda_j^0 + s_{1_j}^1 = 0, \forall \ \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2_j}^1} =$	$-s_j^0 + s_{2_j}^1 = 0, \forall \ \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1L_k}^1} =$	$-\lambda_{L_k}^0 + s_{1L_k}^1 = 0, \forall \ \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2L_k}^1} =$	$-s_{L,k}^0 + s_{2L_k}^1 = 0, \forall \ \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1U_k}^1} =$	$-\lambda_{U_k}^0 + s_{1U_k}^1 = 0, \forall \ \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2U_k}^1} =$	$-s_{U_k}^0 + s_{2U_k}^1 = 0, \forall \ \ k \in K$
2nd level complementarity conditions	Bounds on Lagrange multipliers and slack variables related to original model constraints	$\lambda_{1_j}^1 \cdot s_{1_j}^1 = 0, \forall \ \ j \in J$
		$\lambda_{2_j}^1 \cdot s_{2_j}^1 = 0, \forall \ \ j \in J$
	Bounds on Lagrange multipliers and slack variables related to lower and upper bound of unmeasured uncertain parameters	$\lambda_{1L_k}^1 \cdot s_{1L_k}^1 = 0, \forall \ \ k \in K$
		$\lambda_{2L_k}^1 \cdot s_{2L_k}^1 = 0, \forall \ \ k \in K$
		$\lambda_{1U_k}^1 \cdot s_{1U_k}^1 = 0, \forall \ \ k \in K$
		$\lambda_{2U_k}^1 \cdot s_{2U_k}^1 = 0, \forall \ \ k \in K$
	Lower bound z_n	$\lambda_{L_n}^1 \cdot s_{L_n}^1 = 0, \forall \ \ n \in N$

Description	*Equations*
Upper bound z_n	$\lambda^1_{U_n} \cdot s^1_{U_n} = 0, \forall \ \ n \in N$
Haar Condition	$\sum_j y_j \leq n_z + 1$

Model variables: unmeasured uncertain parameter θ_u, control and state variables z, measured uncertain parameters θ_m, and fixed design variables d. Additional variables: slack variables s, nonnegative λ and free μ Lagrange multipliers.

Note: complementarity conditions are replaced by mixed-integer constraints as described by Eq. (111) and (112).

7. Numerical Examples

The proposed formulations are illustrated in the following examples. In Sections 7.1 to 7.4, the general case formulation is applied and compared against cases with different degrees of control. On the one hand, the case where control actions can compensate for variations of all uncertain parameters is considered, namely the traditional flexibility analysis. On the other hand, the no-recourse case is considered, like the static robust optimization. The solution of the proposed formulations lies between these two extremes. In addition, we include the results for the special case formulations described in Section 3 and the alternative formulation for the general case described in Section 5.

The specific results for each case then involve the following equations:

- Traditional Flexibility Analysis: *(PA1)*.
- Original Formulation of Extended Flexibility Anaysis: *(P9)* for reduced models and *(PC1)* for non-reduced models.
- Alternative Formulation of Extended Flexibility Anaysis: *(PB1)* for reduced models and *(P11)* for non-reduced models.
- Vertex Enumertation for extended flexibility analysis: Eq. (32)
- Upper bound formulation: *(P5)*.
- No control: *(PA2)*.

Moreover, a computational framework has been developed to automatically perform the proposed reformulations. For more details, the reader is referred to Appendix D.

7.1. Linear Example 2

The following example for a flexibility test comprised of three constraints, one control variable, z, two unmeasured uncertain parameters, θ_1 and θ_2, and one measured uncertain parameter θ_3. The example was adapted from Rooney and Biegler (2003).

$$f_1 = z + d_1 - 3d_2 - \theta_1 + 0.5 \cdot \theta_2 + 2 \cdot \theta_3 - 8 \leq 0 \tag{116}$$

$$f_2 = -z + d_2 - \frac{\theta_1}{3} - \theta_2 - \frac{\theta_3}{2} - \frac{8}{3} \leq 0 \tag{117}$$

$$f_3 = z - d_1 + \theta_1 - \theta_2 - \theta_3 - 4 \leq 0 \tag{118}$$

$$11.8907 \leq \theta_1 \leq 18.1093 \tag{119}$$

$$7.29714 \leq \theta_2 \leq 12.0729 \tag{120}$$

$$10 \leq \theta_3 \leq 20 \tag{121}$$

where the design variables are fixed d_1=33.866 and d_2=22.429, corresponding to a feasible design. The solution of the extended flexbility analysis has to lie between u=-4.07, corresponding to the Traditional Flexibility Analysis (TFA) solution, and u=4.19, corresponding to the no control case solution. When we apply the upper bound reformulation, even though a conservative solution is obtained (u=-3.04), the flexibility can be ensured over the entire range of variation of the uncertain parameters as the value of u is negative. The worst constraint violation obtained with the vertex enumeration strategy corresponds to u=-4.07. This value coincides with the solution obtained by applying the original and alternative extended flexibility analysis formulations, and the traditional flexibility analysis formulation. The resulting MINLP from the original EFA formulation takes shorter computational time (0.332 s) than the one resulting from the alternative EFA formulation (1.13 s). The computational results are shown in Table 5.

Table 4. Numerical results of the flexibility test for Linear Example 2.

<table>
<tr><td rowspan="2"></td><td rowspan="2">Traditional Flexibility Analysis</td><td colspan="7">Extended Flexibility Analysis</td><td rowspan="2">No Control</td></tr>
<tr><td>Original Formulation</td><td>Alternative Formulation</td><td colspan="4">Vertex Enumeration for θ_u</td><td>Upper Bound</td></tr>
<tr><td></td><td>$\theta_m = \{\theta_1, \theta_2, \theta_3\}$</td><td colspan="2">$\theta_u = \{\theta_1, \theta_2\}$ $\theta_m = \{\theta_3\}$</td><td colspan="5">$\theta_u^{fixed} = \{\theta_1, \theta_2\}$ $\theta_m = \{\theta_3\}$</td><td>$\theta_u = \{\theta_1, \theta_2, \theta_3\}$</td></tr>
<tr><td>u</td><td>-4.07</td><td>-4.07</td><td>-4.07</td><td>-4.07</td><td>-5.11</td><td>-4.28</td><td>-8.42</td><td>-3.04</td><td>4.19</td></tr>
<tr><td>θ_1</td><td>11.89</td><td>11.891</td><td>11.891</td><td>θ_1^{LB}</td><td>θ_1^{LB}</td><td>θ_1^{UB}</td><td>θ_1^{UB}</td><td>*</td><td>12.927</td></tr>
<tr><td>θ_2</td><td>7.30</td><td>7.30</td><td>7.30</td><td>θ_2^{LB}</td><td>θ_2^{UB}</td><td>θ_2^{LB}</td><td>θ_2^{UB}</td><td>*</td><td>7.927</td></tr>
<tr><td>θ_3</td><td>20</td><td>20</td><td>20</td><td>20</td><td>20</td><td>20</td><td>20</td><td>20</td><td>10</td></tr>
<tr><td>y_1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>0</td><td>0</td><td>1</td><td>0</td></tr>
<tr><td>y_2</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td><td>1</td></tr>
<tr><td>y_3</td><td>0</td><td>0</td><td>0</td><td>0</td><td>0</td><td>1</td><td>1</td><td>0</td><td>0</td></tr>
<tr><td>z</td><td>5.28</td><td>5.28</td><td>5.28</td><td>5.28</td><td>2.18</td><td>3.41</td><td>3.41</td><td>4.24</td><td>0^{**}</td></tr>
</table>

Orig: original reformulation, Alt: alternative formulation, (*) θ_u fixed depending on the sign of the derivative. (**) z fixed to 0 for the no control case.

Table 5. Computational statistics and model size of example 2.

	Traditional Flexibility Analysis	*Extened Flexibility Analysis*							*No Control*
		Original Formulation	*Alternative Formulation*	*Vertex Enumeration for θ_u*				*Upper bound*	
#bin var.	3	35	23	3	3	3	3	3	3
#cont. var.	15	154	91	13	13	13	13	13	11
#constraints	19	156	93	15	15	15	15	15	14
Problem	MILP	MINLP		MILP					
Time [s]	0.100	0.332	1.13	0.093	0.087	0.125	0.094	0.239	0.222
Solver	CPLEX	BARON		CPLEX					

Big M value: 500; solver tolerance: 1E-5, $0 \leq z \leq 6$.

7.2. Heat Exchanger Network Example

A well-known example in the flexibility analysis literature is the heat exchanger network, shown in Figure 1 (Saboo, Morari and Woodcock 1985). Grossmann and Floudas (1987) used this example to introduce the active set strategy, which is able to find non-vertex solutions. After the elimination of the state variables, the reduced model consists of four constraints, and three variables: the cooling load (Q_c) is the control variable, and the heat capacity flowrate of streams 1 and 2 (F_{H1} and F_{H2}) are the uncertain parameters specified over the bounds 1≤ F_{H1} ≤1.8 and 1.95≤ F_{H2} ≤2.05.

$$f_1(z,\theta_1,\theta_2) = 350 - 170 \cdot \theta_2 + z - 195 \cdot \theta_1 + 85 \cdot \theta_2\, \theta_1 - 0.5 \cdot z\, \theta_1 \leq 0 \quad (122)$$

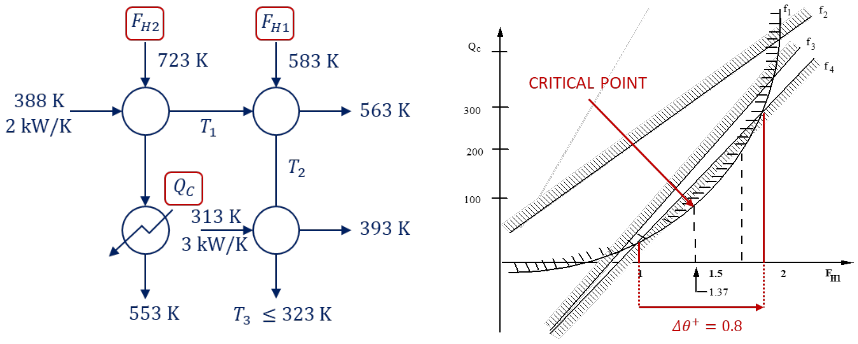
$$f_2(z,\theta_1,\theta_2) = -195 \cdot \theta_1 + 350 - 170 \cdot \theta_2 + z \leq 0 \quad (123)$$

$$f_3(z,\theta_1,\theta_2) = -270 \cdot \theta_1 + 590 - 170 \cdot \theta_2 + z \leq 0 \quad (124)$$

$$f_4(z,\theta_1,\theta_2) = 260 \cdot \theta_1 - 590 + 170 \cdot \theta_2 - z \leq 0 \quad (125)$$

$$0 \leq z \leq 300 \quad (126)$$

where control variable z is the cooling load (Q_c), and the uncertain parameters θ are the heat capacity flowrate of stream H1 (F_{H1}) and H2 (F_{H2}).



(*a*) (*b*)

Figure 7. (a) Heat exchanger network scheme. (b) Feasibility diagram for fixed value of F_{H2}=2.

We solve a modified version of the flexibility test problem for the different cases. Numerical results of the HEN example are summarized in Table 6. As we can see, we obtain positive values of u for all the cases, indicating an infeasible design. Once again, the worst constraint violation is found when no recourse actions are applied (u=185). The value of the worst constraint violation can be reduced to a certain degree when control variables can compensate for the variations in θ_1(u=20). Furthermore, this can be reduced when recourse actions can compensate for variation in both uncertain parameters like in the traditional flexibility analysis (u=7.08). It is also important to note, that non-vertex critical points are obtained for TFA and EFA cases.

Table 6. Numerical results of the flexibility test of the heat exchanger network example.

	Traditional Flexibility Analysis	*Extended Flexibility Analysis*			*No Control*
		Original Formulation	*Alternative Formulation*	*Upper bound*	$\theta_u = \{\theta_1, \theta_2\}$
	$\theta_m = \{\theta_1, \theta_2\}$	$\theta_m = \theta_1$ $\theta_u = \theta_2$		$\theta_m = \theta_1$ $\theta_u^{fixed} = \theta_2$	
u	7.08	20	20	11.07	185.5
θ_1	1.398	1.333	1.333	1.373	1.708
θ_2	1.951	2.05	2.002	*	1.95
y_1	1	1	1	1	0
y_2	0	0	0	0	0
y_3	0	1	1	0	0
y_4	1	0	0	1	1
z	98.21	138.5	130.37	104.46	0^{**}

(*) θ_u fixed depending on the sign of the derivative. (**) z fixed to 0 for the no control case.

Table 7. Computational statistics and model size of heat exchanger network example.

	Traditional Flexibility Analysis	*Extended Flexibility Analysis*			*No Control*
		Original Formulation	*Alternative Formulation*	*Upper bound*	
#bin var.	4	36	20	4	4
#cont. var.	17	161	78	16	12
#constraints	20	163	80	18	10
Time [s]	0.315	2.632	3.362	0.266	0.203

Big M value: 500; solver: BARON, solver tolerance: 1E-2, $0 \leq z \leq 300$

The HEN is a nonlinear programming problem and whose variation with respect to θ_u is not monotonic, therefore we cannot ensure that the worst constraint violation for θ_u will lie at a vertex of the uncertanty set and the application of the upper bound formulation (Section 3.4) can yield to invalid results. As we can see in Table 6, the special case formulation provides a smaller constraint violation (u=11.07) than the actual solution obtained with the original and alternative EFA formulations (u=20). The actual solution is a non-vertex one, that is the reason why it cannot be found by applying the special case, because it simplifies the problem by fixing the value of θ_u to one of its vertex.

The computational results are shown in Table 7.The MINLP problems are solved with BARON 18.5.8 (Kilinc and Sahinidis 2018) and the MILP are solved with CPLEX 12.8.0.0 (IBM ILOG CPLEX Optimization Studio 2018) with default options in an Intel i7 machine with 16 Gb of RAM.

7.3. De-protection Reaction Example

A thermal deprotection reaction is performed in a CSTR, such that the protecting group is cleaved from the protected material (A) to produce the desired product (P) and a gaseous byproduct (BP). The deprotection reaction is performed in tetrahydrofuran (THF). Assume that reaction pressure can be controlled to ensure a single phase in the reactor. The conversion of the protected material (A) needs to be higher than 98%. THF is fully removed in an evaporator by almost fully drying the system and adding the right amounts of two other solvents, butanol and water. The stream leaving the evaporator feeds a crystallizer used to purify the product P. For this final crystallization step, the concentration of P in the crystallizer needs to be less than the solubility of that compound at the boiling point of the mixture butanol/water mixture at atmospheric pressure to ensure full dissolution of the product. Also, the concentration of the product needs to be higher than the solubility at the seed point (T_{seed}) to ensure seed survival and proper purification. It is also desired to maintain the process throughput of at least 1 Kg/day leaving the evaporator.

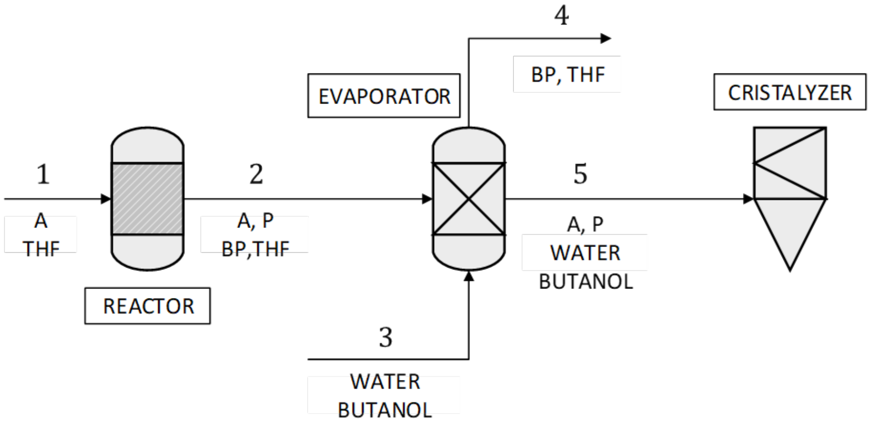


Figure 8. Scheme of de-protection reaction process.

The reaction mechanism follows first order kinetics:

$$\mathrm{A} \overset{\mathrm{k}}{\rightarrow} \mathrm{P} + \mathrm{BP} \tag{127}$$

$$k = A \cdot \exp -E_a/RT_1 \tag{128}$$

$$A^N - \sigma_A \leq A \leq A^N + \sigma_A \tag{129}$$

$$E_a^N - \sigma_{E_a} \leq E_a \leq E_a^N + \sigma_{E_a} \tag{130}$$

where A is the pre-exponential factor [min^{-1}] and E_a is the activation energy [J/mol]. Both A and E_a are considered unmeasured uncertain parameters in the extended flexibility analysis, whose nominal values are 4.2E17 and 1.205E5, respectively; and their variance are 2.4617E13 and 200, respectively. It is important to note that these parameters and their variance have been scaled in the numerical implementation. The measured uncertain parameters are described in Table 8 together with their nominal value and expected deviation. Finally, the control actions are the water and butanol flowrates.

Table 8. Description of measured uncertain parameters.

	Description	*Nominal Value*	*±Expected Deviation*
T_1	Reactor Temperature [K]	353.15	10
V_1	Reaction Volume [L]	50	5
M_1	Reactor Inlet Flowrate [g/min]	89	5
$w_{A,1}$	Inlet Mass Fraction of reactant A	0.07	0.005

The solubility constraints are described with Eqs. (131) and (132).

$$\ln(w_p) \le A_s + \frac{B_s}{T_{boiling}} + C_s \cdot w_{H_2O} + D \cdot \frac{w_{H_2O}}{T_{boiling}} \tag{131}$$

$$\ln(w_p) \ge A_s + \frac{B_s}{T_{seed}} + C_s \cdot w_{H_2O} + D \cdot \frac{w_{H_2O}}{T_{seed}} \tag{132}$$

where $T_{boiling}$ is 366.15 [K] and T_{seed} is 343.15 [K] ; w_p and w_{H_2O} are the weight fraction of product and water, respectively.

As shown in Table 9, we apply the different flexibility test formulations for the non-reduced model to the de-protection reaction example. It is interesting to note that, it is possible to achieve feasible operation for all cases (negative values of u), even when control actions are not allowed as it can be seen in Table 9. Regarding the unmeasured uncertain parameters $\theta_u = \{A, E_a\}$, the worst realization correspond to the lower bound of the pre-exponential factor A and the upper bound of the activation energy E_a, resulting in a slower reaction rate. Regarding the measured uncertain parameters, a lower reaction temperature (343.15 vs. 353 K) also reduces the reaction rate and a smaller reaction volume (45 vs. 50 L) affects the consumption and generation term in the reactor mass balance. However, the effect of the inlet mass flowrate and inlet mass fraction is not completely intuitive, where an increase of these parameters would benefit the minimum conversion and minimum production constraints, but it would also jeopardize the solubility constraints. The computational constraints are shown in Table 10.

Table 9. Numerical results of the flexibility test of the de-protection reaction example.

	Traditional Flexibility Analysis $\theta_m = \theta$	*Extended Flexibility Analysis*		*No Control* $\theta_u = \theta$
		Original Formulation	*Alternative Formulation*	
		$\theta_u = \{A, E_a\}$		
u	-9.96 E-3	-9.96 E-3	-9.80 E-3	-8.8 E-3
A	4.1998 E17	4.1998 E17	4.1998 E17	4.1998 E17
E_a	1.207 E5	1.207 E5	1.207 E5	1.207 E5
T_1	343.15	343.15	343.15	343.15
V_1	45	45	45	45
M_1	92.505	92.505	94	84
$w_{A,1}$	0.065	0.065	0.075	0.074
Active Set	Min conversion Lower bound of solubility Min production	Min convertion Upper and lower bounds of solubility	Min conversion Upper and lower bounds of solubility	Min production

Table 10. Computational statistics and model size of de-protection reaction example.

	Traditional Flexibility Analysiis	*Extended Flexibility Analysis*		*No Control*
		Original Formulation	*Alternative Formulation*	
#bin var.	4	44	28	4
#cont. var.	46	221	128	28
#constraints	53	212	130	34
Time[s]	0.17	0.260	0.150	0.1*
Gap	Rel: 1E-6	Rel: 1E-6	Rel: 1E-6	Abs: 0.988

Big M value: 500; solver: BARON, solver tolerance: 1 E-6, (*) time to find the best solution, max time: 1000, Rel: relative gap, Abs: absolute gap.

7.4. Methanol Synthesis Example

In this section, we evaluate the flexibility of the optimal solution of methanol synthesis problem obtained by Turkay and Grossmann (1996). We consider that the process design consists of reactor, flash, recycle and purge as shown in Figure 9. The objective of the process is to produce at most 1000 tons/day methanol with 90% of purity. It is necessary to purge the inert by-product methane from the recycle stream.

The inlet flowrate, F_{in}[kg-mol/s], is the measured uncertain parameter and the conversion of hydrogen, $conv$, is the unmeasured uncertain parameter. Control variables involve the splitting fraction, E; flash temperature, T_{flsh} [100 K]; and the vapour phase recovery of hydrogen in the flash, $e_{flsh_{H_2}}$. State variables are the components stream flowrate, $fc_{j,i}$ [kg-mol$_i$/s], consumption rate of key component, $consum$ [kg-mol$_{H2}$/s], vapor pressure of individual components, vp_i [MPa], and the vapor phase recovery in the flash for the rest of components, $e_{flsh,i}$ $\{i = CO, CH_3OH, CH_4\}$.

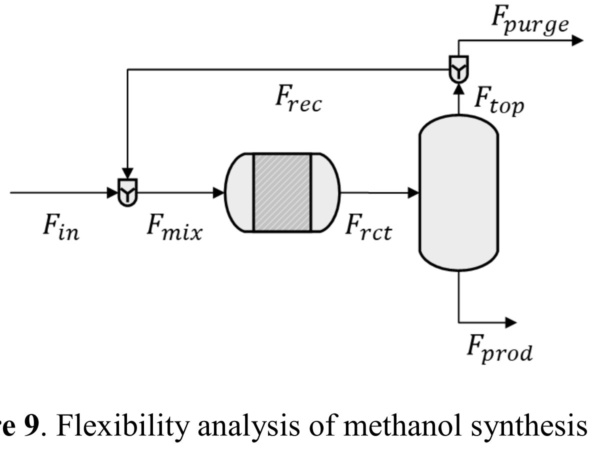


Figure 9. Flexibility analysis of methanol synthesis process.

The inlet stream is described by Eq. (133).

$$fc_{in,i} = F_{in} \cdot Feed_i, \qquad \forall\, i \in I \tag{133}$$

where $i = \{H_2, CO, CH_3OH, CH_4\}$ is the set of chemical components and $Feed_i$ is the feed composition parameter. Eqs. (134) to (136) describe component mass balances of mixer and splitter.

$$fc_{mix,i} = fc_{in,i} + fc_{rec,i}, \qquad \forall\, i \in I \tag{134}$$

$$fc_{rec,i} = E \cdot fc_{top,i}, \qquad \forall\, i \in I \tag{135}$$

$$fc_{ftop,i} = fc_{rec,i} + fc_{purge,i}, \qquad \forall\, i \in I \tag{136}$$

Eqs. (137) and (138) represent the reaction and the mass balance in the reactor.

$$consum = conv \cdot fc_{mix,H_2} \tag{137}$$

$$fc_{rct,i} = fc_{mix,i} + \nu_i \cdot consum, \qquad \forall\, i \in I \tag{138}$$

where H_2 is considered the key component.
The mass balance in the flash separator, Antoine's equation, and recovery and equilibrium relationships are described by Eqs. (139) to (143), respectively.

$$fc_{rct,i} = fc_{ftop,i} + fc_{prod,i}, \qquad \forall\, i \in I \tag{139}$$

$$\log(7500\, vp_i) = A_i - \frac{B_i}{100\, T_{flsh} - C_i}, \qquad \forall\, i \in I \tag{140}$$

$$vp_{H_2} \cdot e_{flsh,i} = e_{flsh,H_2}\left(e_{flsh,i} \cdot vp_{H_2} + \left(1 - e_{flsh,i}\right) \cdot vp_i\right), \qquad \forall\, i \in I \setminus \{H_2\} \tag{141}$$

$$fc_{ftop,i} = e_{flsh,i} \cdot fc_{rct,i}\,, \qquad \forall\, i \in I \tag{142}$$

$$fc_{prod,i} = (1 - e_{flsh,i}) \cdot fc_{rct,i}\,, \qquad \forall\, i \in I \tag{143}$$

Process specifications involve purity of component C constraint (Eq. (144)) and maximum and minimum production constraint (Eq. (145)).

$$fc_{prod,CH_3OH} \geq purity \cdot \sum_i fc_{prod,i} \tag{144}$$

$$minprod \leq \sum_i fc_{prod,i} \leq maxprod \tag{145}$$

We also take into account bounds on flowrates, consumption, partial pressures, fractions and temperatures.

$$fc^{mix} \leq fc_i \leq fc^{max}, \qquad \forall\, i \in I \tag{146}$$

$$0 \leq consum \leq consum^{max} \tag{147}$$

$$vp_i^{min} \leq vp_i \leq vp_i^{max}, \qquad \forall\, i \in I \tag{148}$$

$$eflsh^{min} \leq eflsh_i \leq eflsh^{max}, \qquad \forall\, i \in I \tag{149}$$

$$E^{min} \leq E \leq E^{max} \tag{150}$$

$$T_{flsh}^{min} \leq T_{flsh} \leq T_{flsh}^{max} \tag{151}$$

The range of variation of measured uncertain and unmeasured uncertain parameters are as follows.

$$F_{in}^N + \Delta F_{in}^- \leq F_{in} \leq F_{in}^N + \Delta F_{in}^+ \tag{152}$$

$$conv^N - \Delta conv^- \leq conv \leq conv^N + \Delta conv^+ \tag{153}$$

where the nominal value of F_{in}^N and $conv^N$ are 3.5 and 0.413, respectively. The positive and negative expected deviation of F_{in} is 20% of the nominal value, whereas the positive and negative expected deviation of $conv$ are zero and 10% of the nominal value, respectively.

We perform the flexibility test for the non-reduced model. First, we calculate the worst constraint violation for the no recourse case and for the traditional flexibility analysis in order to obtain an upper and a lower bound of the solution of the extended flexibility analysis, which correspond to 1.91 and -0.01, respectively, as seen in Table 11. This implies that feasible operation cannot be ensured for the range of variation of the inlet flowrate and conversion if no recourse actions are taken, whereas feasible operation can be ensured if control actions can compensate for variations in both uncertain parameters. Then, we apply the original (PC1) and alternative (P11) reformulation of the extended flexibility test for non-reduced models to the methanol synthesis problem. As a result, we obtain a value of u of 0.48 for the original and alternative reformulations. Therefore, feasible operation cannot be ensured for the range of variation of both parameters if control actions are restricted to compensate only for variations in the measured uncertain parameters. The computational results are shown in Table 12.

Table 11. Numerical results of the flexibility test for the methanol synthesis example.

	Traditional Flexibility Analysis $\theta_m = \{F_{in}, conv\}$	*Extended Flexibility Analysis* *Original Formulation*	*Alternative Formulation*	*No Control* $\theta_u = \{F_{in}, conv\}$
		$\theta_m = F_{in}$ $\theta_u = conv$		
u	-0.01	0.48	0.48	1.91
F_{in}	4.2	4.2	4.2	4.2
$conv$	0.37	0.37	0.37	0.37
Active Set	e^{max}_{flsh,H_2} T^{min}_{flsh} $purity$ $max\,prod$ fc^{max}_{mix,H_2}	$vp^{max}_{CH_4}$ $purity$ $max\,prod$ fc^{max}_{mix,H_2}	$vp^{max}_{CH_4}$ $purity$ $max\,prod$ fc^{max}_{mix,H_2}	fc^{max}_{mix,H_2}

Table 12. Computational statistics and model size of methanol synthesis example.

	Traditional Flexibility Analysis	*Extended Flexibility Analysis* *Original Formulation*	*Alternative Formulation*	*No Control*
#bin var.	33	201	93	27
#cont. var.	128	913	370	69
#constraints	133	903	363	71
Time [s]	0*	155.16*	77.44*	0.150
Gap	Abs: 0.32	Rel: 0.75	Rel: 0.75	0

Big M value: 500, solver: BARON, solver tolerance: 1E-2, (*) time to find the best solution, max time: 1000, Rel: relative gap, Abs: absolute gap

The last two examples correspond to MINLP problems, which are solved with BARON 19.3.24 (Kilinc and Sahinidis 2018) in an Intel i7 machine with 16 Gb of RAM. The Vertex enumeration for θ_u method and upper bound formulations are not applied, as monotonicity of the unmeasured uncertain with respect to model constraint parameters cannot be proved.

It is worth noting that for the special cases, where the single level formulation is similar to the one obtained with the TFA. The same restrictions apply in order to obtain a global solution. The approach guarantees global optimality to a restricted set of problems where the flexibility constraints $\chi(d)$ are quasi-concave in θ_m and the constraint functions are jointly quasi-concave in z and θ_m and strictly quasi-convex in z for fixed θ_m. In order to obtain global solution for a non-convex problem, a solution strategy as proposed by Floudas *et al*. (2001) should be followed.

For the general case formulation, the KKT conditions for non-covex problem only represent the necessary optimality conditions and may lead to local solutions. Therefore, we emphasize the need of providing the tightest bounds to all type of variables and establishing the lower and upper bound of the extended flexibility problem with the solutions from the traditional flexibility analysis and the case of no control, respectively.

Conclusions

The traditional flexibility analysis has been extended in order to obtain more accurate results when dealing with operation under uncertainty, where a distinction of the uncertain parameters is made between the measured and unmeasured uncertain parameters. In this work, we have proposed new MINLP reformulations of the resulting multilevel optimization problem, which involve replacing the innermost problem by its KKT optimality conditions in a recursive fashion and the introduction of a mixed-integer representation of the complementarity conditions.

We have demonstrated that the formulation can be simplified for special cases, such as convex problems, problems whose constraints vary monotonically with respect to the measured and unmeasured uncertain parameters and with respect to the unmeasured uncertain parameters only. A feature of the first two cases is that the worst constraint violation lies at a vertex of the uncertain parameter sets, where the solution can be obtained via vertex enumeration. In such cases, it is proved that the solution can be obtained by applying the traditional flexibility analysis.

For the third case, a vertex enumeration method for the unmeasured uncertain parameters together with the active set method at each vertex of T_u can be applied to find the solution of the extended flexibility test. In addition, an upper bound formulation is proposed, leading to a similar formulation as the one obtained by applying the active set constraint strategy (Grossmann and Floudas, 1987).

For the general case, we have proposed two MINLP reformulations. The original reformulation involves the replacement of the inner problems by their optimality and complementarity conditions three times, whereas in the alternative reformulation, an interchange of the order of the innermost maximization problems results in the replacement of the inner problems by their optimality and complementarity conditions only twice. This modification results in a final model of smaller size. We have also extended the formulations to include models with equality constraints.

The reformulations were successfully tested and compared in six examples, including three analytical examples, a heat exchanger network, a de-protection reaction and a simplified flowsheet for methanol synthesis.

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Appendix A: Review of Traditional Flexibility Analysis

As shown by Grossmann and Floudas (1987) the flexibility test can be reformulated in the following MINLP:

$$(PA1): \chi(d) = \max_{\theta \in T} u$$

$$s.t. \quad \theta^{LB} \leq \theta \leq \theta^{UB}$$

$$1 - \sum_j \lambda_j^0 = 0$$

$$\sum_j \lambda_j^0 \cdot \frac{\partial f_j}{\partial z} = 0$$

$$f_j(d, z, \theta) - u + s_j^0 = 0, \qquad \forall \ j \in J$$

$$\lambda_j^0 - y_j^0 \leq 0, \qquad \forall \ j \in J$$

$$s_j^0 - M\left(1 - y_j^0\right) \leq 0, \qquad \forall \ j \in J$$

$$\sum_j y_j^0 \leq n_z + 1$$

$$\lambda_j^0, s_j^0 \ \geq 0, y_j^0 \in \{0,1\}, \qquad \forall \ j \in J$$

If there are no recourse variables the flexibility test reduces to:

$$(PA2): \chi(d) = \max_{\theta \in T} u$$

$$s.t. \quad \theta^{LB} \leq \theta \leq \theta^{UB}$$

$$f_j(d, \theta) - u + s_j^0 = 0, \qquad \forall \ j \in J$$

$$s_j^0 - M\left(1 - y_j^0\right) \leq 0, \qquad \forall \ j \in J$$

$$\sum_j y_j^0 = 1$$

$$s_j^0 \ \geq 0, y_j^0 \in \{0,1\}, \qquad \forall \ j \in J$$

Appendix B: Alternative Reformulation of Extended Flexibility Analysis of Reduced Models

Table B1 Alternative reformulation of reduced models.

Description		*Equations*
Objective function	$(PB1)$:	$\chi(d) = \max_{\theta_m \in T_m} \psi(d, \theta_m)$
Model constraints	$\frac{\partial \mathcal{L}_1}{\partial \mu_{1_j}^1} = \frac{\partial \mathcal{L}_0}{\partial \lambda_j^0} =$	$f_j(d, z, \theta_m, \theta_u) - u + s_j^0 = 0, \forall \ \ j \in J$
1st level complementarity conditions	Model constraints	$\lambda_j^0 \cdot s_j^0 = 0, \forall \ \ j \in J$
	Lower bound θ_u	$\lambda_{L_k}^0 \cdot s_{L_k}^0 = 0, \forall \ \ k \in K$
	Upper bound θ_u	$\lambda_{U_k}^0 \cdot s_{U_k}^0 = 0, \forall \ \ k \in K$
Derivatives w.r.t. original model variables	$\frac{\partial \mathcal{L}_1}{\partial \mu_{5_k}^1} = \frac{\partial \mathcal{L}_0}{\partial \theta_{u_k}} =$	$\sum_j \lambda_j^0 \frac{\partial f_j}{\partial \theta_{u_k}} - \lambda_{L_k}^0 + \lambda_{U_k}^0 = 0, \forall \ \ k \in K$
Lower bound θ_u	$\frac{\partial \mathcal{L}_1}{\partial \mu_{6_k}^1} =$	$\theta_{u_k}^{LB} - \theta_{u_k} + s_{L_k}^0 = 0, \ \ k \in K$
Upper bound θ_u	$\frac{\partial \mathcal{L}_1}{\partial \mu_{7_k}^1} =$	$\theta_{u_k} - \theta_{u_k}^{UB} + s_{U_k}^0 = 0, \ \ k \in K$
Derivatives w.r.t. original model variables	$\frac{\partial \mathcal{L}_1}{\partial u} =$	$1 - \sum_j \mu_{1_j}^1 - \sum_n (\lambda_{L_n}^1 + \lambda_{U_n}^1) = 0$
	$\frac{\partial \mathcal{L}_1}{\partial z_n} =$	$\sum_j \mu_{1_j}^1 \cdot \frac{\partial f_j}{\partial z_n} + \sum_k \mu_{5_k}^1 \sum_j \lambda_j^0 \frac{\partial^2 f_j}{\partial z_n \partial \theta_{u_k}} - \lambda_{L_n}^1 + \lambda_{U_n}^1 = 0$ $\forall \ \ n \in N$
	$\frac{\partial \mathcal{L}_1}{\partial \theta_{u_k}} =$	$\sum_j \mu_{1_j}^1 \cdot \frac{\partial f_j}{\partial \theta_{u_k}} + \sum_{k'} \mu_{5_{k'}}^1 \sum_j \lambda_j^0 \frac{\partial^2 f_j}{\partial \theta_{u_k} \partial \theta_{u_{k'}}}$ $- \mu_{6_k}^1 + \mu_{7_k}^1 = 0, \qquad \forall \ \ k \in K$
Derivatives w.r.t. slack variable	$\frac{\partial \mathcal{L}_1}{\partial s_j^0} =$	$\mu_{1_j}^1 + \mu_{2_j}^1 \cdot \lambda_j^0 - \lambda_{2_j}^1 = 0, \forall \ \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial s_{L_k}^0} =$	$\mu_{4_k}^1 \cdot \lambda_{L_k}^0 + \mu_{6_k}^1 - \lambda_{2L_k}^1 = 0, \forall \ \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial s_{U_k}^0} =$	$\mu_{3_k}^1 \cdot \lambda_{U_k}^0 + \mu_{7_k}^1 - \lambda_{2U_k}^1 = 0, \forall \ \ k \in K$

Description	Equations	
Derivatives w.r.t. Lagrange multiplier of previous level	$\frac{\partial \mathcal{L}_1}{\partial \lambda_j^0} =$	$\mu_{2_j}^1 \cdot s_j^0 + \sum_k \mu_{5_k}^1 \frac{\partial f_j}{\partial \theta_{u_k}} - \lambda_{1_j}^1 = 0, \forall \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{L_k}^0} =$	$\mu_{4_k}^1 \cdot s_{L_k}^0 - \mu_{5_k}^1 - \lambda_{1L_k}^1 = 0, \forall \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{U_k}^0} =$	$\mu_{3_k}^1 \cdot s_{U_k}^0 + \mu_{5_k}^1 - \lambda_{1U_k}^1 = 0, \forall \ k \in K$
Lower bound z_n	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{L_n}^1} =$	$-z_n + z_n^{LB} + s_{L_n}^1 - u = 0, \forall \ n \in N$
Upper bound z_n	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{U_n}^1} =$	$z_n - z_n^{UB} + s_{U_n}^1 - u = 0, \forall \ n \in N$
Bounds on Lagrange multipliers and slack variables	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1_j}^1} =$	$-\lambda_j^0 + s_{1_j}^1 = 0, \forall \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2_j}^1} =$	$-s_j^0 + s_{2_j}^1 = 0, \forall \ j \in J$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1L_k}^1} =$	$-\lambda_{L_k}^0 + s_{1L_k}^1 = 0, \forall \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2L_k}^1} =$	$-s_{L,k}^0 + s_{2L_k}^1 = 0, \forall \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{1U_k}^1} =$	$-\lambda_{U_k}^0 + s_{1U_k}^1 = 0, \forall \ k \in K$
	$\frac{\partial \mathcal{L}_1}{\partial \lambda_{2U_k}^1} =$	$-s_{U_k}^0 + s_{2U_k}^1 = 0, \forall \ k \in K$
2nd level complementarity conditions	Bounds on Lagrange multipliers and slack variables related to model constraints	$\lambda_{1_j}^1 \cdot s_{1_j}^1 = 0, \forall \ j \in J$
		$\lambda_{2_j}^1 \cdot s_{2_j}^1 = 0, \forall \ j \in J$
	Bounds on Lagrange multipliers and slack variables related to lower and upper bound of unmeasured uncertain parameters	$\lambda_{1L_k}^1 \cdot s_{1L_k}^1 = 0, \forall \ k \in K$
		$\lambda_{2L_k}^1 \cdot s_{2L_k}^1 = 0, \forall \ k \in K$
		$\lambda_{1U_k}^1 \cdot s_{1U_k}^1 = 0, \forall \ k \in K$
		$\lambda_{2U_k}^1 \cdot s_{2U_k}^1 = 0, \forall \ k \in K$
	Lower bound z_n	$\lambda_{L_n}^1 \cdot s_{L_n}^1 = 0 \ \forall \ n \in N$
	Upper bound z_n	$\lambda_{U_n}^1 \cdot s_{U_n}^1 = 0 \ \forall \ n \in N$
Haar Condition	$\sum_j y_j \leq n_z + 1$	

Model variables: unmeasured uncertain parameter θ_u, control variables z, measured uncertain parameters θ_m, and fixed design variables d. Additional variables: slack variables s, nonnegative λ and free μ Lagrange multipliers.

Note: complementarity conditions are replaced by mixed-integer constraints as described by Eq. (111) and (112).

Appendix C: Original Reformulation of Extended Flexibility Analysis of Non-Reduced Models

Table C 1. Original reformulation of non-reduced models

Description		*Equation*
Objective function	$(PC1)$:	$\chi(d) = \max_{\theta_m \in T_m} u$
Model equality constraints	$\frac{\partial \boldsymbol{\mathcal{L}_2}}{\partial \boldsymbol{\mu^2_{0_i}}} = \frac{\partial \boldsymbol{\mathcal{L}_1}}{\partial \boldsymbol{\mu^1_{0_i}}} = \frac{\partial \boldsymbol{\mathcal{L}_0}}{\partial \boldsymbol{\mu^0_i}} =$	$\boldsymbol{h_i(d, z, \theta_m, \theta_u) = 0}, \quad \forall \ \boldsymbol{i \in I}$
Model inequality constraints	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{1_j}} = \frac{\partial \mathcal{L}_1}{\partial \mu^1_{1_j}} = \frac{\partial \mathcal{L}_0}{\partial \lambda^0_j} =$	$g_j(d, z, \theta_m, \theta_u) - u + s^0_j = 0, \quad \forall \ j \in J$
Derivatives w.r.t. Lagrange multiplier of outermost level	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_3} = \frac{\partial \mathcal{L}_1}{\partial \mu^1_3} = \frac{\partial \mathcal{L}_0}{\partial u} =$	$1 - \sum_j \lambda^0_j = 0$
	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_4} = \frac{\partial \mathcal{L}_1}{\partial u} =$	$-1 - \sum_j \mu^1_{1_j} = 0$
	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{5_k}} = \frac{\partial \mathcal{L}_1}{\partial \theta_{u_k}} =$	$\sum_j \mu^1_{1_j} \frac{\partial g_j}{\partial \theta_{u_k}} + \sum_{\boldsymbol{i}} \boldsymbol{\mu^1_{0_i}} \frac{\partial \boldsymbol{h_i}}{\partial \boldsymbol{\theta_{u_k}}} - \lambda^1_{3_k} + \lambda^1_{4_k} = 0 \quad \forall \, k \in K$
	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{6_j}} = \frac{\partial \mathcal{L}_1}{\partial s^0_j} =$	$\mu^1_{1_j} + \mu^1_{2_j} \cdot \lambda^0_j - \lambda^1_{2_j} = 0\,, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{7_j}} = \frac{\partial \mathcal{L}_1}{\partial \lambda^0_j} =$	$\mu^1_{2,j} \cdot s^0_j - \mu^1_3 - \lambda^1_{1_j} = 0, \quad \forall \ j \in J$
Lower bound θ_u	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{12_k}} =$	$\theta^{LB}_{u_k} - \theta_{u_k} + s^1_{3_k} = 0, \quad \forall \ k \in K$
Upper bound θ_u	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{13_k}} =$	$\theta_{u_k} - \theta^{UB}_{u_k} + s^1_{4_k} = 0, \quad \forall \ k \in K$
Bounds on Lagrange multipliers and slack variables	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{8_j}} = \frac{\partial \mathcal{L}_1}{\partial \lambda^1_{1_j}} =$	$-\lambda^0_j + s^1_{1_j} = 0, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial \mu^2_{9_j}} = \frac{\partial \mathcal{L}_1}{\partial \lambda^1_{2_j}} =$	$-s^0_j + s^1_{2_j} = 0, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial \lambda^2_{1_j}} =$	$-\lambda^1_{1_j} + s^2_{1j} = 0, \quad \forall \ j \in J$

Description	*Equation*
	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{2_j}^2} = \quad -\lambda_{2_j}^1 + s_{2j}^2 = 0, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{5_k}^2} = \quad -\lambda_{3_k}^1 + s_{5_k}^2 = 0, \quad \forall \ k \in K$
	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{7_k}^2} = \quad -\lambda_{4_k}^1 + s_{7_k}^2 = 0, \quad \forall \ k \in K$
Bounds on Lagrange multipliers and slack variables	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{3_j}^2} = \quad -s_{1_j}^1 + s_{3_j}^2 = 0, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{4_j}^2} = \quad -s_{2_j}^1 + s_{4_j}^2 = 0, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{6_k}^2} = \quad -s_{3_k}^1 + s_{6_k}^2 = 0, \quad \forall \ k \in K$
	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{8_k}^2} = \quad -s_{4_k}^1 + s_{8_k}^2 = 0, \quad \forall \ k \in K$
Lower bound z_n	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{9_n}^2} = \quad -z_n + z_n^{LB} + s_{9_n}^2 - u = 0, \quad \forall \ n \in N$
Upper bound z_n	$\frac{\partial \mathcal{L}_2}{\partial \lambda_{10_n}^2} = \quad z_n - z_n^{UB} + s_{10_n}^2 - u = 0, \quad \forall \ n \in N$
	$\frac{\partial \mathcal{L}_2}{\partial u} = \quad 1 - \sum_j \mu_{1_j}^2 - \sum_n (\lambda_{9_n}^2 + \lambda_{10_n}^2) = 0$
Derivatives w.r.t. model variables	$\frac{\partial \mathcal{L}_2}{\partial \theta_{u_k}} = \quad \sum_j \mu_{1_j}^2 \frac{\partial g_j}{\partial \theta_{u_k}} + \sum_{\boldsymbol{i}} \boldsymbol{\mu_{0_i}^2} \frac{\boldsymbol{\partial h_i}}{\boldsymbol{\partial \theta_{u_k}}} + \sum_{k'} \mu_{5_{k'}}^2 \left(\sum_j \mu_{1_j}^1 \frac{\partial^2 g_j}{\partial \theta_{u_k} \partial \theta_{u_{k'}}} + \sum_{\boldsymbol{i}} \boldsymbol{\mu_{0_i}^1} \frac{\boldsymbol{\partial^2 h_i}}{\boldsymbol{\partial \theta_{u_k} \partial \theta_{u_{k'}}}} \right) - \mu_{12_k}^2 + \mu_{13_k}^2 = 0, \quad \forall \ k \in K$
	$\frac{\partial \mathcal{L}_2}{\partial z_n} = \quad \sum_j \mu_{1_j}^2 \frac{\partial g_j}{\partial z_n} + \sum_{\boldsymbol{i}} \boldsymbol{\mu_{0_i}^2} \frac{\boldsymbol{\partial h_i}}{\boldsymbol{\partial z_n}} + \sum_k \mu_{5_k}^2 \left(\sum_j \mu_{1_j}^1 \frac{\partial^2 g_j}{\partial z_n \, \partial \theta_{u_k}} + \sum_{\boldsymbol{i}} \boldsymbol{\mu_{0_i}^1} \frac{\boldsymbol{\partial^2 h_i}}{\boldsymbol{\partial z_n \, \partial \theta_{u_k}}} \right) - \lambda_{9_n}^2 + \lambda_{10_n}^2 = 0, \quad \forall \ n \in N$
Derivatives w.r.t. slack variable	$\frac{\partial \mathcal{L}_2}{\partial s_j^0} = \quad \mu_{1_j}^2 + \mu_{2_j}^2 \cdot \lambda_j^0 + \mu_{7_j}^2 \cdot \mu_{2_j}^1 - \mu_{9_j}^2 = 0, \quad \forall \ j \in J$
	$\frac{\partial \mathcal{L}_2}{\partial s_{1_j}^1} = \quad \mu_{8_j}^2 + \mu_{10_j}^2 \cdot \lambda_{1_j}^1 - \lambda_{3_j}^2 = 0, \quad \forall \ j \in J$

Description		*Equation*
	$\dfrac{\partial \mathcal{L}_2}{\partial s^1_{2_j}} =$	$\mu^2_{9_j} + \mu^2_{11_j} \cdot \lambda^1_{2_j} - \lambda^2_{4_j} = 0, \quad \forall \ j \in J$
	$\dfrac{\partial \mathcal{L}_2}{\partial s^1_{3_k}} =$	$\mu^2_{14_k} \cdot \lambda^1_{3_k} - \lambda^2_{6_k} + \mu^2_{12_k} = 0, \quad \forall \ k \in K$
	$\dfrac{\partial \mathcal{L}_2}{\partial s^1_{4_k}} =$	$\mu^2_{15_k} \cdot \lambda^1_{4_k} - \lambda^2_{8_k} + \mu^2_{13_k} = 0, \quad \forall \ k \in K$
Derivatives w.r.t. multipliers of previous levels	$\dfrac{\partial \mathcal{L}_2}{\partial \lambda^0_j} =$	$\mu^2_{2_j} \cdot s^0_j - \mu^2_3 + \mu^2_{6_j} \cdot \mu^1_{2_j} - \mu^2_{8_j} = 0, \quad \forall \ j \in J$
	$\dfrac{\partial \mathcal{L}_2}{\partial \lambda^1_{1_j}} =$	$-\mu^2_{7_j} + \mu^2_{10_j} \cdot s^1_{1_j} - \lambda^2_{1_j} = 0, \quad \forall \ j \in J$
	$\dfrac{\partial \mathcal{L}_2}{\partial \lambda^1_{2_j}} =$	$-\mu^2_{6_j} + \mu^2_{11_j} \cdot s^1_{2_j} - \lambda^2_{2_j} = 0, \quad \forall \ j \in J$
	$\dfrac{\partial \mathcal{L}_2}{\partial \lambda^1_{3_k}} =$	$\mu^2_{14_k} \cdot s^1_{3,k} - \lambda^2_{5_k} = 0, \quad \forall \ k \in K$
	$\dfrac{\partial \mathcal{L}_2}{\partial \lambda^1_{4_k}} =$	$\mu^2_{15_k} \cdot s^1_{4_k} - \lambda^2_{7_k} = 0, \quad \forall \ k \in K$
	$\boldsymbol{\dfrac{\partial \mathcal{L}_2}{\partial \mu^1_{0_i}}} =$	$\boldsymbol{\sum_k \mu^2_5 \cdot \dfrac{\partial h_i}{\partial \theta_{u,k}} = 0}, \quad \forall \ \boldsymbol{i \in I}$
	$\dfrac{\partial \mathcal{L}_2}{\partial \mu^1_{1_j}} =$	$-\mu^2_4 + \sum_k \mu^2_5 \cdot \dfrac{\partial g_j}{\partial \theta_{u_k}} + \mu^2_{6_j} = 0, \quad \forall \ j \in J$
	$\dfrac{\partial \mathcal{L}_2}{\partial \mu^1_{2_j}} =$	$\mu^2_{6_j} \cdot \lambda^0_j + \mu^2_{7_j} \cdot s^0_j = 0, \quad \forall \ j \in J$
	$\dfrac{\partial \mathcal{L}_2}{\partial \mu^1_3} =$	$-\sum_j \mu^2_{7_j} = 0$
1st level complementarity conditions	Model constraints	$\lambda^0_j \cdot s^0_j = 0, \quad \forall \ j \in J$
2nd level complementarity conditions	Bounds on Lagrange multipliers and slack variables related to model constraints	$\lambda^1_{1_j} \cdot s^1_{1_j} = 0, \quad \forall \ j \in J$ $\lambda^1_{2_j} \cdot s^1_{2_j} = 0, \quad \forall \ j \in J$
	Lower bound θ_u	$\lambda^1_{3,k} \cdot s^1_{3,k} = 0, \quad \forall \ k \in K$
	Upper bound θ_u	$\lambda^1_{4,k} \cdot s^1_{4,k} = 0, \quad \forall \ k \in K$
3rd level complementarity conditions	Bounds on Lagrange multipliers and slack variables related to original model constraints	$\lambda^2_{l_j} \cdot s^2_{l_j} = 0, \quad \forall \ j \in J, \ l = \{1, \dots, 4\}$

Description		Equation	
	Bounds on Lagrange multipliers and slack variables related to lower and upper bound of unmeasured uncertain parameters	$\lambda_{l_k}^2 \cdot s_{l_k}^2 = 0,$	$\forall \ k \in K,$ $l = \{5, \dots, 8\}$
	Lower bound z_n Upper bound z_n	$\lambda_{l_n}^2 \cdot s_{l_n}^2 = 0\,,$	$\forall \ n \in N,$ $l = \{9, 10\}$
Haar Condition		$\sum_j y_j \leq n_z + 1$	

Model variables: unmeasured uncertain parameter θ_u, control and state variables z, measured uncertain parameters θ_m, and fixed design variables d.
Additional variables: slack variables s, nonnegative λ and free μ Lagrange multipliers.

Note: complementarity conditions are replaced by mixed-integer constraints as described by Eq. (111) and (112).

Appendix D: Computational Software

A great challenge involved in the flexibility analysis problems is the reformulation of the rigorous mathematical formulations for these problems that include non-conventional max-min-max and max-min-max-max optimization problems, which cannot be readily solved with standard optimization techniques. In general, these types of reformulations are implemented manually and are then tedious, time-consuming and error prone. In order to avoid these drawbacks, we have developed a tool that automatically performs the reformulation of the flexibility problem (Deshpande 2018), based on a widely used open source algebraic modeling language, Pyomo (Hart, et al. 2017), written in the high level programming language Python.
The tool comprises of a Python module file that contains the flexibility analysis function. The arguments of the function are the model equations and constraints of the system under study, a list of the measured and unmeasured uncertain parameters and their expected positive and negative deviation, and a list of the control variables together with their lower and upper bounds. Once the reformulation is automatically developed within the module, it is solved by using an appropriate MINLP solver, which returns the flexibility test results, along with critical values of the uncertain parameters. In addition, we use the python interface to GAMS 25.1.2 (GAMS Development Corporation 2018) solvers.

Nomenclature Section

Reformulations

Subscripts
Inequality constraints, j
Unmeasured uncertain parameters, k
Control variables, n
Superscripts
Upper bound, UB
Lower bound, LB
First optimization level, 0
Second optimization level, 1
Third optimization level, 2
Sets
Set of inequality reduced constraints, J
Set of unmeasured uncertain parameters, K
Set of control variables, N
Variables
Design variables, d
Control variables, z
Uncertain parameters, θ
Measured uncertain parameters, θ_m
Unmeasured uncertain parameters, θ_u
Scalar variable of worst constraint violation, u
Nonnegative Lagrange multipliers / slack variables

- Original model constraints, λ_j^0/s_j^0
- Bounds on Lagrange multiplier of 1st level, $\lambda_{1_j}^1/\ s_{1_j}^1$
- Bounds on slack variables of 1st level, $\lambda_{2_j}^1/, s_{2_j}^1$
- Lower bound of unmeasured uncertain parameters, $\lambda_{3_k}^1/s_{3_k}^1$
- Upper bound of unmeasured uncertain parameters, $\lambda_{4_k}^1/s_{4_k}^1$
- Bounds on Lagrange multiplier of 2nd level, $\lambda_{1_j}^2/s_{1_j}^2$; $\lambda_{2_j}^2/, s_{2_j}^2$; $\lambda_{5_k}^2/s_{5_k}^2$; $\lambda_{7_k}^2/s_{7_k}^2$
- Bounds on slack variables of 2nd level, $\lambda_{3_j}^2/s_{3_j}^2$; $\lambda_{4_j}^2/, s_{4_j}^2$; $\lambda_{6_k}^2/\ s_{6_k}^2$; $\lambda_{8_k}^2/s_{8_k}^2$
- Lower bound of control variables, $\lambda_{9_n}^2/s_{9_n}^2$
- Upper bound of control variables, $\lambda_{10_n}^2/s_{10_n}^2$

Free Lagrange multipliers

- Second level:
  - Model equality constraints, $\mu_{1_j}^1$
  - Complementarity conditions of original model constraints, $\mu_{2_j}^1$
  - Necessary condition$\partial\mathcal{L}_0/\partial u$, μ_3^1
- Third level:
  - Model equality constraints, $\mu_{1_j}^2$
  - Complementarity conditions:
    - Original model constraints $\mu_{2_j}^2$
    - Bound in Lagrange multiplier, $\mu_{10_j}^2$

Bound in slack variable, $\mu^2_{11_j}$

Lower bound of unmeasured uncertain parameters, $\mu^2_{14_k}$

Upper bound of unmeasured uncertain parameters, $\mu^2_{15_k}$

Necessary conditions:

$\partial\mathcal{L}_1/\partial\mu^1_3$, μ^2_3

$\partial\mathcal{L}_1/\partial u$, μ^2_4

$\partial\mathcal{L}_1/\partial\theta_{u_k}$, $\mu^2_{5_k}$

$\partial\mathcal{L}_1/\partial s^0_j$ $\mu^2_{6_j}$

$\partial\mathcal{L}_1/\partial\lambda^0_j$, $\mu^2_{7_j}$

Bounds in nonnegative Lagrange multipliers and slack variables, $\mu^2_{8_j}$, $\mu^2_{9_j}$

Lower and upper bound of unmeasured uncertain parameters, $\mu^2_{12_k}$, $\mu^2_{13_k}$

Binary variables to model the choice of the active set, y^0_j

Expressions

Flexibility constraint, χ

Lagrangean function, $\mathcal{L}$

Inequality reduced constraints, f

Inequality constraints, g

Equality constraints, h

Optimization problems, ψ, ζ, ϕ,

Parameters

Coefficients of linear terms, a_j, b_j, c_j, d_j

Big M value, M

Dimension of the control variable, n_z

Lower and upper bound of unmeasured uncertain parameters, $\theta^{LB}_{u_k}$, $\theta^{UB}_{u_k}$

Lower and upper bound control variables, z^{LB}_n, z^{UB}_n

De-protection Reaction Example

Sets:

Set of streams, $j = \{1, 2, 3, 4, 5\}$

Set of chemical components, $i = \{A, P, BP, THF, H_2O, B\}$

Fixed Parameters

Solubility constants, A_S:13.303, B_S:-5946.878, C_S:-31.909, D_S:12881.683

Seed Temperature [K], T_{seed}: 343.15

Boiling Temperature [K], $T_{boiling}$: 366.15

Molecular weight [g_i/mol_i],

$MW_i = \{A{:}470, P{:}\ 370, BP{:}100, THF{:}72.11, H_2O{:}18.02, B{:}74.12\}$

Density [g_i/ml], $\rho_i = \{A{:}1, P{:}\ 1, BP{:}1, THF{:}0.889, H_2O{:}1, B{:}0.810\}$

Variables:

Components stream molar flowrate [mol_i/min], $f_{i,j}$ (0; 200)

Components stream mass flowrate [g_i/min], $m_{i,j}$ (0; 200)

Total stream mass flowrate [g/min], M_j (0; 500)

Mass fraction [g_i/g], $w_{i,j}$ (0; 1)

Volumetric flowrate of reactor inlet stream [L/min], v_0 (0.001; 200)

Reactor inlet and outlet concentration of reactive A [mol_A/L], $C_{A,1}$, $C_{A,2}$ (0.001;1)

Reaction constant [min^{-1}], k

Reaction rate [mol/(min L)], r

Control Variables:

Water and butanol inlet stream mass flowrate [g_i/min], $m_{i,j}$, $i = \{H_2O, B\}$, $j = 3$, (5; 90)

Measured uncertain parameters:

Reactor temperature [K], T_1

Reaction volume [L], V_1

Total mass flowrate of reactor inlet stream [g/min], M_1

Mass fraction of reactive A reactor inlet stream [g_i/g], $w_{A,1}$

Unmeasured uncertain parameters:

Pre-exponential factor [min^{-1}], A

Activation energy [J/mol], E_a

Methanol Synthesis Example

Sets:

Set of streams, $j = \{in, mix, rct, ftop, rec, prod, purge\}$

Set of chemical components, $i = \{H_2, CO, CH_3OH, CH_4\}$

Variables:

Components stream flowrate [kg-mol_i/s], $fc_{j,i}$ (0; 5)

Consumption rate of key component [kg-mol_{H2}/s], $consum$ (0; 5)

Splitting fraction, E (0.01; 0.99)

Flash temperature [100 K], T_{flsh} (3.4; 5)

Vapor pressure of individual components [MPa], vp_i ($vp_i^{min}(T_{flsh}^{min})$; $vp_i^{max}(T_{flsh}^{max})$)

Vapor phase recovery in flash, $e_{flsh,i}$ (0.1; 0.99)

Parameters

Feed composition, $Feed_i$ = {H_2: 0.65, CO: 0.30, CH_3OH: 0, CH_4: 0.05}

Stoichiometry coefficient, ν_i {H_2: -1, CO: -0.5, CH_3OH: 0.5, CH_4: 0}

Antoine coefficients

A_i = {H_2: 13.6333, CO: 14.3686, CH_3OH: 18.5875, CH_4: 15.2243}

B_i = {H_2: 164.9, CO: 530.22, CH_3OH: 3626.55, CH_4: 897.84}

C_i = {H_2: 3.19, CO: -13.15, CH_3OH: -34.29, CH_4: -7.16}

Measured uncertain parameters:

Inlet flowrate [kg-mol/s], F_{in}

Unmeasured uncertain parameters:

Conversion of key component, $conv$