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

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Abstract

In this paper, we formulate the flexibility analysis with measured and unmeasured parameters as a rigorous multi-level optimization problem. First, we propose to recursively reformulate the inner optimization problems by the Karush-Kuhn-Tucker conditions and with a mixed-integer representation of the complementarity conditions to solve the resulting multilevel optimization problem. Three types of problems are addressed and solved with the proposed strategy: 1) linear programming problem, 2) nonlinear programming problem with monotonic variation of unmeasured uncertain, and finally 3) nonlinear programming problem. We illustrate the new formulations with a heat exchanger network problem with uncertain heat capacity flowrates.

Keywords: extended flexibility analysis, optimization under uncertainty, MINLP formulation.

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 guaranteed feasibility of operation of a plant over a range of conditions, with the ultimate goal being on how to design a process for guaranteed flexible operation (Grossmann *et al*., 2014). The flexibility test problem only determines whether a design 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 such that the model inequalities hold over the uncertain parameter range (Swaney and Grossmann, 1985).

However, these formulations are based on the assumption that manipulated variables can compensate for any variation in the uncertain parameter set and 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 analysis by taking into account the level of parametric uncertainty in the mathematical models at the operation stage, by grouping the uncertain parameters, $\theta \in \Theta$, into two types, measured and unmeasured parameters. The flexibility constraint was then extended to account for model parameters, θ_u, that cannot be measured.

In this paper, we propose a new reformulation of the extended flexibility analysis where the innermost problems are recursively replaced by their optimality conditions and the complementarity conditions are expressed with a discrete representation.

2. Mathematical Model

The basic model for the flexibility analysis involves design variables, d, control variables, z, and uncertain parameters, θ. One of the main problems addressed in the flexibility analysis is the flexibility test problem. It consists in determining whether by proper adjustment of the control variables the process constraints $g_j(d,z,\theta) \le 0$, $j \in J$, hold for any realization of uncertain parameters for a given design (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).

$$\forall \theta \in \Theta \{\exists z\ (\forall j \in J\ [g_j(d,z,\theta) \le 0])\} \tag{1}$$

$$\leftrightarrow \chi(d) = \max_{\theta \in \Theta} \min_{z} \max_{j \in J} g_j(d,z,\theta) \tag{2}$$

The main difference between the design and control variables is that the design variables are fixed during the operation stage, while the control variables can be adjusted in order to satisfy process constraints. In fact, to solve the flexibility constraint it is required to have accurate estimation of the uncertain parameters. This can only be achieved if there is enough process data for precise determination of all uncertain parameter values. However, this assumption is restrictive, and 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 to 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. The second group includes the unmeasured uncertain parameters, θ_u, whose estimation cannot be performed during the operation stage, consequently no control actions can be applied to them.

This distinction has been taken into account and the flexibility constraint was then extended to Eq. (3) and reformulation as the multilevel optimization problem described by Eq. (4) by Ostrovsky *et al.* (2003) and Rooney and Biegler (2003).

$$\forall \theta_m \in \Theta_m \{\exists z\ (\forall \theta_u \in \Theta_u, \forall j \in J\ [g_j(d,z,\theta_m,\theta_u) \le 0])\} \tag{3}$$

$$\leftrightarrow \chi(d) = \max_{\theta_m \in \Theta_m} \min_{z} \max_{\theta_u \in \Theta_u} \max_{j \in J} g_j(d,z,\theta_m,\theta_u) \tag{4}$$

To solve the extended flexibility analysis, Ostrosvky *et al*. (2003) suggested an algorithm for calculation of the flexibility function based on the 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 involved the use of the KS smooth function (Krelsselmeler and Steinhauser, 1983) that aggregated 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 resulted in a nonlinear program.

In this work, we reformulate the extended flexibility constraint by developing the optimality conditions for each nested problems. 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 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 derivate the formulation of three different cases, linear problem, non-linear problem with monotonic variation of unmeasured parameters with respect to model constraints, and non-linear problems.

2.1. Special Case 1: Linear Programming problem

The order of the inner max operators in Eq. (4), are interchangeable and can be equivalently expressed as follows.

$$\begin{aligned}
&\chi(\mathrm{d}) = \max_{\theta_m \in \Theta_m} \psi(\mathrm{d},\theta_m) \\
&\quad s.t\ \ \psi(\mathrm{d},\theta_m) = \min_{z} \zeta(\mathrm{d},\mathrm{z},\theta_m) \\
&\qquad\quad s.t.\ \ \zeta(\mathrm{d},\mathrm{z},\theta_m) = \max_{j\in J} \max_{\theta_u \in \Theta_u} \mathrm{g}_j(\mathrm{d},\mathrm{z},\theta_m,\theta_u)
\end{aligned} \tag{5}$$

We consider that the inner problem is described by the linear inequality constraints:

$$\mathrm{g}_j(\mathrm{d},\mathrm{z},\theta_m,\theta_u) = \mathrm{a}_j \cdot d + b_j \cdot z + c_j \cdot \theta_u + d_j \cdot \theta_m \le 0, \forall j \in J \tag{6}$$

Constraints g_j in Eq. (6) vary monotonically with respect to θ_u. Hence, the solution of the innermost problem must lie in one of the extreme points of its range of variation, depending on the sign of the derivative, $dg_j/d\theta_{j,u}$.

$$\max_{\theta_u \in \Theta_u} \mathrm{g}_j(\theta_{j,u}) \rightarrow \theta^*_{j,u} \tag{7}$$

The bilevel problem M1 described by Eq. (8) is obtained by replacing Eq. (7) in Eq. (5). To obtain a single level optimization problem, the innermost problem of Eq. (8) is replaced by its optimality conditions with a mixed integer representation of the complementarity condition following the active constraint set strategy (Grossmann and Floudas, 1987). This yields the MILP problem:

$$\begin{aligned}
&\mathrm{M1}: \chi(\mathrm{d}) = \max_{\theta_m \in \Theta_m} \psi(\mathrm{d},\theta_m) \\
&\quad s.t.\ \psi(\mathrm{d},\theta_m) = \min_{z,u}\left(u \,\middle|\, \mathrm{g}_j(\mathrm{d},\mathrm{z},\theta_m,\theta_u) = \mathrm{a}_j \cdot d + b_j \cdot z + c_j \cdot \theta^*_{j,u} + d_j \cdot \theta_m \le u, \forall j \in J\right)
\end{aligned} \tag{8}$$

Where u is a scalar variable that represents the worst constraint violation.

2.2. Special Case 2: Non-Linear Programming problem with monotonic variation of unmeasured uncertain parameters

If the set of functions $g_j(d,z,\theta_m,\theta_u)$ varies monotonically with respect to the unmeasured uncertain parameters, then the relationship expressed by Eq. (7) holds true. Therefore, the solution of the innermost problem lies at an extreme point of the range of variation of θ_u. Analogously, the following bilevel programming problem M2 is obtained and then reformulated in the same way as the previous case, but leading to the MINLP problem.

$$\begin{aligned} &\mathrm{M2}: \chi(\mathrm{d}) = \max_{\theta_m \in \Theta_m} \psi(\mathrm{d},\theta_m) \\ &\quad s.t{:}\ \psi(\mathrm{d},\theta_m) = \min_{z,u}(u \,|\, \mathrm{g}_j(\mathrm{d,z},\theta_m,\theta^*_{j,u}) \le u, \forall j \in J) \end{aligned} \tag{9}$$

2.3. General Case: Non-Linear Programming problem

The extended flexibility constraint can be equivalently expressed as the following multi-level optimization problem M3.

$$\begin{aligned} &\mathrm{M3}: \chi(\mathrm{d}) = \max_{\theta_m \in \Theta_m} \psi(\mathrm{d},\theta_m) \\ &\quad s.t\ \ \psi(\mathrm{d},\theta_m) = \min_{z} \zeta(\mathrm{d,z},\theta_m) \\ &\quad s.t{:}\ \zeta(\mathrm{d,z},\theta_m) = \max_{\theta_u \in \Theta_u} \varphi(\mathrm{d,z},\theta_m,\theta_u) \\ &\quad\ \ s.t{:}\ \ \varphi(\mathrm{d,z},\theta_m,\theta_u) = \min_{u}(u \,|\, \mathrm{g}_j(\mathrm{d,z},\theta_m,\theta_u) \le u, \forall j \in J) \end{aligned} \tag{10}$$

In order to solve Eq. (10), we propose to replace the inner problems by their optimality conditions in a recursive fashion. Due to space limitations, we cannot report the complete reformulation. To illustrate the solution strategy, we will replace the innermost problem of Eq. (10) by its KKT conditions (Eqns. (11) and (12)) and complementarity conditions (Eq. (13)). Bounds of the Lagrange multipliers, λ_j^0, and slack variables, s_j^0, are added as model constraints of the next level optimization problem, described by Eqns. (14) and (15), in order to tighten the formulation.

$$1\text{-}\sum_j \lambda_j^0 = 0 \tag{11}$$

$$\mathrm{g}_j(\mathrm{d,z},\theta_m,\theta^*_{j,u})\text{-}u + s_j^0 = 0 \qquad \forall j \in J \tag{12}$$

$$\lambda_j^0 \cdot s_j^0 = 0 \qquad \forall j \in J \tag{13}$$

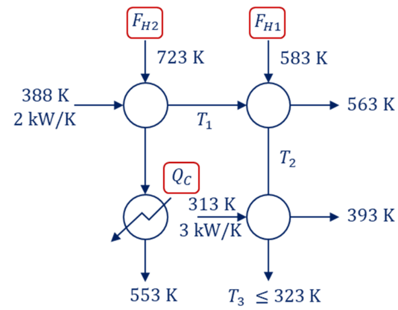
$$-\lambda_j^0 \le 0 \qquad \forall j \in J \tag{14}$$

$$-s_j^0 \le 0 \qquad \forall j \in J \tag{15}$$

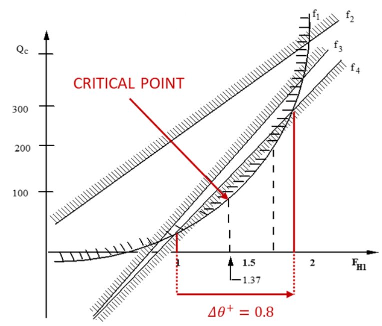
Following this procedure, we obtain a single level optimization problem. The complementarity conditions are then expressed with a mixed integer representation, the Haar conditions is assumed, leading to an MINLP problem.

3. Numerical Example

A well-known example in the flexibility analysis literature is the heat exchanger network, shown in Figure 1. 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. We solve a modified version the problem for three cases. First, considering both uncertain parameters as unmeasured, so no recourse actions can be taken. Second, considering θ_1 as a measured uncertain parameter and θ_2 as an unmeasured uncertain parameter, where control actions can only be adjusted to compensate for variations in θ_1, solved with the proposed formulation. Finally, we consider both as measured uncertain parameters like in the traditional flexibility analysis.



(*a*)



(*b*)

Figure 1. (*a*) Heat exchanger network scheme. (*b*) Feasibility diagram for fixed value of F_{H2}=2

Numerical results are summarized in Table 1Table 1. As we can see, we obtain positive values of u for all the cases, indicating an infeasible design. The worst constraint violation (u=138.5) is obtained for the case of no recourse actions. This value can be reduced up to certain degree (u=20) when control variables can compensate for the variations in θ_1. Furthermore, this can be reduced (u=7.08) when recourse actions can compensate for variation in both uncertain parameters. It is also important to note, that non-vertex critical points are obtained for the second and third cases. The different problems are implemented in GAMS 25.1.2 (GAMS Development Corporation, 2018) and solved with BARON 18.5.8 (Kilinc and Sahinidis, 2018) in an Intel i7 machine with 16 Gb of RAM. The tolerance of the solver is set to 0.01 and the big M value is 600.

Table 1. Worst constraint violation, critical parameters values for three examples and model size.

	Both unmeasured uncertain parameters* θ_u=θ_1, θ_2	Combined type of uncertain Parameters θ_m=θ_1,θ_u=θ_2	Both measured uncertain Parameters θ_m=θ_1, θ_2
u	138.5	20	7.08
θ_1= F_{H1}	1	1.333	1.398
θ_2= F_{H2}	1.95	2.041	2.034
#bin var	4	36	6
#cont. var	12	161	22
#constraints	13	163	21
CPU time	0.01	1.67	0.09

*For a fixed value of z.

4. Conclusion

In order to obtain more realistic results when dealing with operation under uncertainty, a distinction of the uncertain parameters can made between the measured and unmeasured uncertain parameters. Thus, the traditional flexibility constraint has been extended. In this work, we have proposed new reformulations of the resulting multilevel optimization problem, which involves the replacement the innermost problem by its optimality conditions in a recursive fashion and the introduction of a mixed-integer representation of the complementarity conditions, resulting in an MINLP problem.

We have developed the formulation of three different cases, linear problem, non-linear problem with monotonic variation of unmeasured parameters with respect to model constraints, and non-linear problems. A particular feature of the first two cases is that the worst constraint violation lies at a vertex of the unmeasured uncertain parameter set; where the formulation can be simplified, leading to a similar formulation as the one obtained by applying the active set constraint strategy, namely the traditional flexibility analysis (Grossmann and Floudas, 1987). An example of a heat exchanger network has been presented to illustrate the proposed reformulation of the general case and compared to cases with different degree of recourse actions.

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