On the Relation Between Flexibility Analysis and Robust Optimization for Linear Systems

Qi Zhang[a], Ricardo M. Lima[b], Ignacio E. Grossmann[a,*]

[a] *Center for Advanced Process Decision-making, Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA*
[b] *Center for Uncertainty Quantification in Computational Science & Engineering, Computer, Electrical and Mathematical Sciences and Engineering Division, King Abdullah University of Science and Technology, Thuwal 23955-6900, Kingdom of Saudi Arabia*

Abstract

Flexibility analysis and robust optimization are two approaches to solving optimization problems under uncertainty that share some fundamental concepts, such as the use of polyhedral uncertainty sets and the worst-case approach to guarantee feasibility. The connection between these two approaches has not been sufficiently acknowledged and examined in the literature. In this context, the contributions of this work are fourfold: (1) a comparison between flexibility analysis and robust optimization from a historical perspective is presented; (2) for linear systems, new formulations for the three classical flexibility analysis problems—flexibility test, flexibility index, and design under uncertainty—based on duality theory and the affinely adjustable robust optimization (AARO) approach are proposed; (3) the AARO approach is shown to be generally more restrictive such that it may lead to overly conservative solutions; (4) numerical examples show the improved computational performance from the proposed formulations compared to the traditional flexibility analysis models.

*Corresponding author
Email address: grossmann@cmu.edu (Ignacio E. Grossmann)

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Introduction

This paper is a tribute to Roger Sargent, the founder and intellectual leader of the area of process systems engineering (PSE), and his pioneering work on design of chemical plants with uncertain parameters,[1] which has inspired many of the later works on flexibility analysis and optimal design under uncertainty.

Process flexibility and resiliency analysis of chemical processes using mathematical optimization models have received significant attention in the PSE community for more than thirty years. In general, the study of the flexibility of a process can be addressed at two stages: (1) at the design stage, where the optimization models for process design explicitly incorporate flexibility constraints, or (2) when for a fixed design, there is the need to evaluate the process flexibility in the presence of perturbations of some operating conditions, which at the design stage were considered constant, but in reality are subject to uncertainty.

In a recent review paper,[2] Grossmann et al. give a historical perspective on the evolution of the concepts and mathematical models used for flexibility analysis. Some of the earlier works in this area include the work of Friedman and Reklaitis[3,4] from the mid 70s, who proposed techniques for solving linear programming (LP) problems with some of the parameters subject to uncertainty; subsequently from the 80s the resiliency concepts proposed by Saboo et al.[5] and applied to heat exchanger networks; and the development of optimization models to quantify process flexibility by solving the flexibility test and flexibility index problems.[6,7]

The analysis of the flexibility of chemical processes is closely related to the solution of optimization problems under uncertainty. In the works mentioned above, one assumes that each uncertain parameter can take any value within a given range, and the process is considered sufficiently flexible if feasible operation can be achieved for the entire parameter range. Interestingly, the exact same idea forms the foundation of robust optimization,[8] which was introduced in the late 90s. The increasing interest in robust optimization in recent years has led to many theoretical developments and its application to a wide range of problems.[9,10]

The two main concepts shared by flexibility analysis and robust optimization are the following:

- using polyhedral uncertainty sets to describe the uncertainty in the parameters;
- applying worst-case analysis to test feasibility.

However, while the most effective solution approaches developed in flexibility analysis make use of the Karush-Kuhn-Tucker (KKT) conditions and insights on the possible sets of active constraints as it is aimed at solving nonlinear models, robust optimization applies duality theory to linear models to obtain tractable formulations.

Another major difference between flexibility analysis and "traditional" robust optimization is the treatment of recourse (reactive actions after the realization of the uncertainty). While flexibility analysis explicitly considers control variables that can adjust depending on the realized values of the uncertain parameters, robust optimization traditionally does not account for recourse, which often leads to overly conservative solutions. This gap between the two approaches is being bridged by the recent development of the adjustable robust optimization concept,[11,12] which allows the incorporation of recourse decisions, typically in the form of linear decision rules.

In this work, we consider a set of linear inequality constraints with a given general structure for which the following three flexibility analysis problems are addressed:

1. the flexibility test problem;
2. the flexibility index problem;
3. design under uncertainty with flexibility constraints.

For linear models described by inequalities, we establish the link between flexibility analysis and robust optimization by first developing a new flexibility analysis approach based on duality. Then, we apply the affinely adjustable robust optimization[11] approach to the same flexibility analysis problems. Hence, we present and compare the following three approaches:

1. traditional (KKT-based) flexibility analysis (TFA);
2. duality-based flexibility analysis (DFA);
3. affinely adjustable robust optimization (AARO).

While the TFA and DFA approaches lead to mixed-integer linear programming (MILP) formulations, only LPs need to be solved in the AARO approach. However, we show that while the TFA and DFA approaches obtain the same optimal solution, the AARO approach may predict a lower level of flexibility due to the restriction of the recourse to linear functions of the uncertain parameters. The performance of the different approaches is demonstrated in several numerical case studies.

The remainder of this paper is organized as follows. In the next section, we give a historical perspective on flexibility analysis and robust optimization, which have been developed independently from each other in different research communities. In the subsequent three sections, the three flexibility analysis problems are introduced, and for each of them, the formulations resulting from the three different solution approaches are presented. These formulations are then applied to three numerical examples. Finally, we close with a summary of the main results and some concluding remarks.

Historical Perspective

While flexibility analysis was developed in the PSE community, robust optimization is recognized as a subfield of operations research (OR). In the following, we take a look at the historical development of these two research areas, which interestingly have evolved almost entirely independently from each other.

In their seminal work from 1975,[3,4] Friedman and Reklaitis address the problem of solving LPs with possibly correlated uncertain parameters, where each uncertain parameter can take any value within a known range of variation. A worst-case approach is proposed which aims at finding a solution that is feasible for any possible realization of the uncertainty. General nonlinear systems are considered in the work by Grossmann and Sargent from 1978,[1] which forms the basis for all later contributions in the area of flexibility analysis. The major conceptual innovation is the distinction between design and control variables; while design variables are chosen at the design stage and cannot be changed during the operation of the plant, control variables can be adjusted depending on the realization of the uncertain parameters. This concept resembles the stage-wise construction of stochastic programming[13] models and realistically represents the decision-making process in chemical plant design and operation.

Most of the later theoretical work in flexibility analysis was conducted in the 1980s by Grossmann and coworkers. Halemane and Grossmann[6] introduce a rigorous formulation of the problem of design under uncertainty. A max-min-max constraint, which involves solving what is known as the flexibility test problem, guarantees the existence of a feasible region for the specified range of parameter values. One main result is that if the constraints are convex, the solution of the flexibility test problem lies at a vertex of the polyhedral region of parameters. Based on this insight, a vertex enumeration formulation and an iterative cutting plane algorithm are proposed to solve the design under uncertainty problem. Swaney and Grossmann[7,14] introduce the flexibility index problem by proposing a quantitative index which measures the size of the parameter space over which feasible operation can be attained. Two algorithms have been proposed that are designed to avoid exhaustive vertex enumeration. Realizing that the flexibility test and flexibility index problems result in bilevel formulations, Grossmann and Floudas[15] replace the lower-level problems by their KKT conditions and apply an active-constraint strategy to convert the bilevel problems into single-level mixed-integer problems. The derivation of the model does not require the assumption of vertex solutions; hence, it is able to predict nonvertex critical points.

Pistikopoulos and Grossmann consider the optimal retrofit design with the objective of improving process flexibility.[16,17] Further extensions include stochastic flexibility,[18,19] where the uncertain parameters are described by a joint probability distribution function; flexibility analysis of dynamic systems;[20] flexible design with confidence intervals and process variability;[21,22] new flexibility measure from constructing feasible polytopes in the parameter space;[23] and simplicial approximation of feasibility limits.[24,25] More recent works focus on data-driven approaches for flexibility analysis.[26,27,28]

While the area of flexibility analysis has evolved over the last 40 years, the history of robust optimization is very different. The work that is generally recognized as the first contribution to the area of robust optimization is a short technical note from 1973 by Soyster,[29] who considers robust solutions to LPs with column-wise uncertainty, which can be seen as a special case of the problem addressed by Friedman and Reklaitis.[3,4] Then, essentially no further development was made in the OR community until Soyster's work was rediscovered in 1998 by Ben-Tal and Nemirovski[30] and El Ghaoui et al.,[31] who introduced the notion of uncertainty sets and robust counterparts. While an uncertainty set is the set of all possible realizations of the uncertainty, a robust counterpart is a formulation that constraints the original model equations to be feasible for every possible realization of the uncertainty.

The major concern in robust optimization is computational tractability which strongly depends on the structure of the optimization problem and the form of the uncertainty set. Tractable robust counterparts have been derived for a wide variety of optimization problems,[8] often by using duality theory. For example, the robust counterpart of an LP with uncertain parameters defined by polyhedral uncertainty sets can be formulated as an LP of similar complexity;[32] the robust counterpart of an LP with ellipsoidal uncertainty can be posed as a second-order cone program (SOCP);[32] and for qudratically constrained quadratic programs (QCQPs) with simple ellipsoidal uncertainty, the robust counterpart is a semidefinite program (SDP).[33] Some of the results for continuous problems can be extended to models with discrete variables.[34] For many other classes of optimization problems, however, only tractable approximate solution approaches have been proposed so far.[31,35,36] In particular, obtaining robust solutions for general nonlinear systems remains a major challenge.

One drawback of robust optimization is that the result may often be overly conservative since the approach optimizes for the worst case. To address this issue, Bertsimas and Sim[37] introduce the notion of a budget of uncertainty, which can be changed in order to adjust the level of conservatism in the solution. In the proposed approach, the budget of uncertainty is encoded in the form of a cardinality constraint on the number of uncertain parameters that are allowed to deviate from their nominal values, and probabilistic bounds for constraint satisfaction as functions of the budget parameter are derived. The concept of probabilistic guarantees in robust optimization traces back to Ben-Tal and Nemirovski,[38] who show that for an ellipsoid with radius Ω, the corresponding robust feasible solution satisfies the original constraint with probability at least $1 - e^{-\Omega^2/2}$. Since then, probabilistic guarantees have been derived for a number of different robust formulations.[39,36,40]

Unlike flexibility analysis, traditional static robust optimization does not consider recourse, which is another limitation that may lead to overly conservative solutions. A more realistic approach has been introduced with the concept of adjustable/adaptable robust optimization,[11,41] which involves adjustable recourse decisions that depend on the realization of the uncertainty. Benders-dual cutting plane[42] and column-and-constraint generation[43,44] algorithms have been proposed to solve the two-stage robust optimization problem with fully adjustable recourse. However, solving fully adjustable robust optimization problems is very difficult and in many cases intractable; an effective way to reduce the computational effort is to describe the recourse decisions as functions of the uncertain parameters and then restrict these functions to specific tractable forms. Several classes of recourse functions have been proposed in the literature,[45,46,47] among which the affine or linear decision rules[11] are most popular. While affine decision rules allow the formulation of efficient multistage models and are shown to be optimal for some specific types of problems,[48,49] they generally form a restriction of the fully adjustable case and hence are suboptimal. Kuhn et al.[12] estimate the approximation error from using linear decision rules by applying them to both the primal and the dual of the problem.

More recent developments in robust optimization include adjustable robust optimization with integer recourse[50,51,52] and distributionally robust optimization,[53,54] which addresses the problem of ambiguity in the probability distribution that describes the uncertain parameters. We refer to recent review papers[9,10] for a more comprehensive overview of the advances made by the OR community in this rapidly growing research area.

In recent years, robust optimization has also been applied by the PSE community, mainly to production scheduling problems[55,56,57,58,59,60,61,62] involving uncertainty in prices, product demands, processing times etc. With only very few exceptions,[63] most works apply the static robust optimization approach without recourse. Gounaris et al.[64] derive robust counterparts for the capacitated vehicle routing problem. Li et al.[65] apply robust optimization to linear and mixed-integer linear optimization problems, and present a systematic study of the robust counterparts for various uncertainty sets and their geometric relationships. In a subsequent work, Li et al.[66] derive probabilistic guarantees for constraint satisfaction when applying these robust counterparts.

In Figure 1, we illustrate the evolution of flexibility analysis and robust optimization over time by showing a timeline with some of the most seminal works from each research area. One can see that flexibility analysis has a much longer history than robust optimization; but interestingly, it is not mentioned in any robust optimization literature. In this work, we show the strong connections between the two approaches, and highlight the fact that some of the fundamental concepts in robust optimization have already been developed in the area of flexibility analysis long before the era of robust optimization.

Furthermore, it is interesting to note that some concepts from flexibility analysis and robust optimization have been independently developed and applied in a third field, namely the field of robust design of mechanical systems.[67,68] In particular, the so-called corner space evaluation method[69] strongly resembles the vertex enumeration method from flexibility analysis.

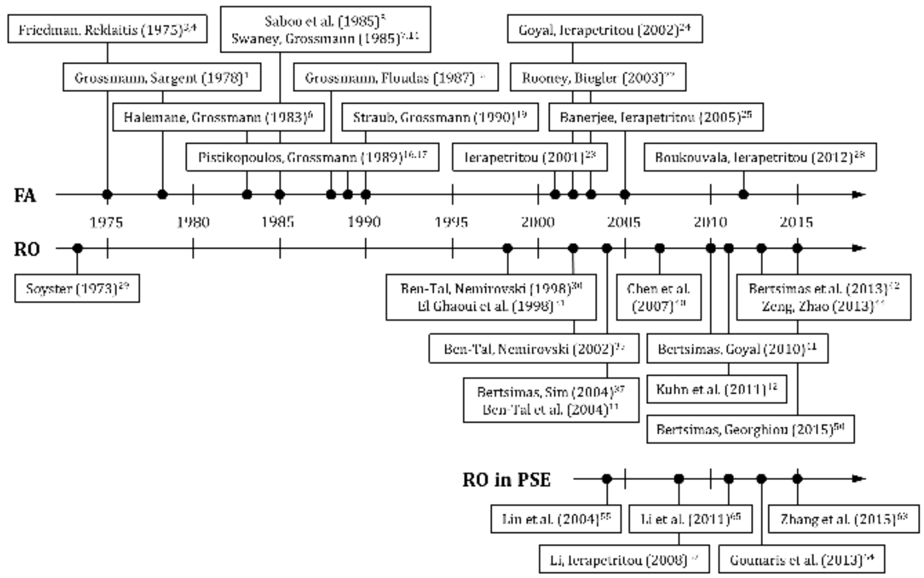


Figure 1: Timeline showing some of the seminal works in flexibility analysis (FA), robust optimization (RO), and robust optimization in PSE.

Flexibility Test Problem

Problem Statement

Consider a set of m linear inequality constraints of the following form:

$$f_j(d, z, \theta) = a_j\, d + b_j\, z + c_j\, \theta \leq 0 \quad \forall\, j \in J \tag{1}$$

where $d \in \mathbb{R}^{n_d}$ are design variables, $z \in \mathbb{R}^{n_z}$ are control variables, and $\theta \in \mathbb{R}^{n_\theta}$ are uncertain parameters; $J = \{1, 2, \ldots, m\}$ is the set of constraints, a_j, b_j, and c_j are row vectors of appropriate dimensionalities. In engineering applications, the inequalities typically represent restrictions on the operating conditions of a process and product requirements. In a general linear model involving equality and inequality constraints, they result from eliminating the state variables from the equations and substituting them in the inequalities. Note that constant summands in the constraint functions can be incorporated in this general formulation by defining fixed dummy design variables.

The flexibility test problem[6] can then be stated as follows: For a given design d, determine whether by proper adjustment of the control variables z, the inequalities $f_j(d,z,\theta) \le 0,\ j \in J$, hold for all $\theta \in T = \left\{\theta : \theta^{\mathrm{L}} \le \theta \le \theta^{\mathrm{U}}\right\}$. Here, T denotes the uncertainty set, which normally takes the form of an n_θ-dimensional hyperbox.

Traditional Flexibility Analysis

For fixed d and θ, the feasibility function is defined as

$$\psi(d,\theta) = \min_{z \in \mathbb{R}^{n_z}} \max_{j \in J} f_j(d,z,\theta) \tag{2}$$

which returns the smallest largest f_j that can be achieved by adjusting z. If $\psi(d,\theta) \le 0$, we can have feasible operation; if $\psi(d,\theta) > 0$, the operation is infeasible regardless how we choose z. $\psi(d,\theta)$ can be obtained by solving the following LP:

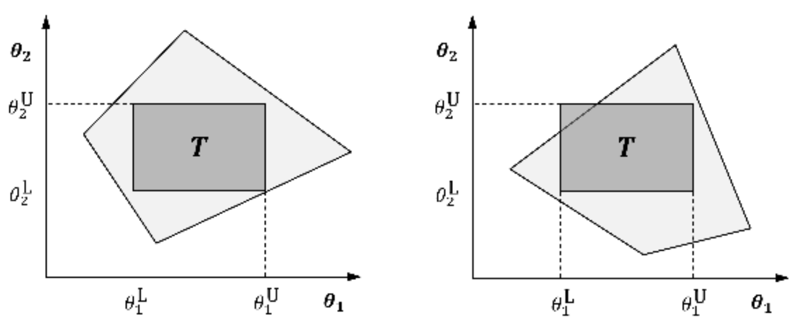
$$\begin{aligned} \psi(d,\theta) = \min_{z,u} \quad & u \\ \text{s.t.} \quad & A\,d + B\,z + C\,\theta \le u\,e \\ & z \in \mathbb{R}^{n_z},\ u \in \mathbb{R}, \end{aligned} \tag{FF}$$

where e denotes a column vector of appropriate dimensionality where all entries are 1.

The flexibility test problem is equivalent to checking whether the maximum value of $\psi(d,\theta)$ is less than or equal to zero over the entire range of θ. Hence, it can be formulated as[6]

$$\chi(d) = \max_{\theta \in T} \psi(d,\theta) = \max_{\theta \in T} \min_{z \in \mathbb{R}^{n_z}} \max_{j \in J} f_j(d,z,\theta) \tag{FT}$$

where $\chi(d)$ corresponds to the flexibility function of design d with respect to the uncertainty set T. The geometric interpretation of the flexibility test problem is illustrated in Figure 2, where for each of the two examples, the feasible region, which is a polyhedron in the $(2+n_z)$-dimensional (θ, z)-space, is projected onto the 2-dimensional θ-space. In the example shown in Figure 2a, the problem is feasible for all $\theta \in T$ as the rectangle describing T is inscribed in the projection of the feasible region, resulting in $\chi(d) \le 0$. In fact, here, $\chi(d) = 0$ since one of the vertices of T touches the boundary of the feasible region. In the second example shown in Figure 2b, the given design is not feasible for all $\theta \in T$ as T is not completely contained in the projection of the feasible region.



(a) Feasible design, $\chi(d) \le 0$ **(b)** Infeasible design, $\chi(d) > 0$

Figure 2: Examples of feasible and infeasible design with respect to a given uncertainty set T.

An important property from flexibility analysis is expressed in the following theorem.[6]

Theorem 1. *If the constraint functions $f_j(d, z, \theta)$ are jointly convex in z and θ, Problem (FT) has its global solution at a vertex of the polyhedral region $T = \left\{\theta : \theta^{\mathrm{L}} \leq \theta \leq \theta^{\mathrm{U}}\right\}$.*

In the case of (1), the constraint functions are clearly jointly convex in z and θ since they only appear linearly in f_j. Hence, we can apply Theorem 1 and solve the flexibility test problem by evaluating $\psi(d, \theta)$ at all vertices of T. Based on this property, Swaney and Grossmann[14] have proposed two solution algorithms (direct search and implicit enumeration), which search over the set of vertices, but are designed to avoid exhaustive enumeration.

The solution approach that we consider here is an active-set method[15] that formulates the flexibility test problem as one single MILP. In this approach, the flexibility test problem given by Eq. (FT) is posed as a bilevel problem in which Problem (FF) is the lower-level problem used to compute $\psi(d, \theta)$. A single-level formulation is achieved by replacing the lower-level problem with its KKT conditions and by modeling the choice of the set of active constraints with mixed-integer constraints. The resulting flexibility test formulation is as follows:

$$
\begin{aligned}
\chi(d) = \max_{\theta,z,u,\lambda,s,y} \quad & u \\
\text{s.t.} \quad & A\,d + B\,z + C\,\theta + s = u\,e \\
& e^{\mathrm{T}}\lambda = 1 \\
& B^{\mathrm{T}}\lambda = 0 \\
& \lambda \le y \\
& s \le M(e - y) \\
& e^{\mathrm{T}} y \le n_z + 1 \\
& \theta \in T,\ z \in \mathbb{R}^{n_z},\ u \in \mathbb{R},\ \lambda \in \mathbb{R}^m_+,\ s \in \mathbb{R}^m_+,\ y \in \{0,1\}^m,
\end{aligned}
\tag{FT$_{\mathrm{TFA}}$}
$$

where s is the vector of slack variables, λ denotes the vector of Lagrange multipliers, and M is a big-M parameter. Note that Problem (FT$_{\mathrm{TFA}}$) has $3m + n_z + 2n_\theta + 2$ constraints, $2m + n_z + n_\theta + 1$ continuous variables, and m binary variables.

Duality-based Flexibility Analysis

We now present an alternative approach, which is derived using LP duality theory and makes use of Theorem 1. First, we define a new uncertainty set that only contains the vertices of T:

$$\overline{T} = \left\{\theta : \theta_i = \theta_i^{\mathrm{N}} + x_i\,\Delta\theta_i^+ - (1 - x_i)\Delta\theta_i^-,\ x_i \in \{0,1\}\ \ \forall\, i \in \Theta\right\} \tag{3}$$

where $\Delta\theta^+ = \theta^{\mathrm{U}} - \theta^{\mathrm{N}}$, $\Delta\theta^- = \theta^{\mathrm{N}} - \theta^{\mathrm{L}}$, and $\Theta = \{1, 2, \ldots, n_\theta\}$ is the set of uncertain parameters. The vertices are expressed by using the binary variables x. If $x_i = 1$,

$\theta_i = \theta_i^{\mathrm{U}}$; otherwise, $\theta_i = \theta_i^{\mathrm{L}}$.

The dual of Problem (FF) is

$$\psi(d,\theta) = \max_{\lambda} \quad (A\,d + C\,\theta)^{\mathrm{T}}\,\lambda \tag{4a}$$

$$\text{s.t.} \quad e^{\mathrm{T}}\lambda = 1 \tag{4b}$$

$$-\,B^{\mathrm{T}}\lambda = 0 \tag{4c}$$

$$\lambda \in \mathbb{R}_{+}^{m}, \tag{4d}$$

where λ is the vector of nonnegative dual variables. Due to strong duality, Problems (FF) and (4) achieve the same objective function value at the optimal solution. Hence, the flexibility test problem can be reformulated as:

$$\chi(d) = \max_{\theta \in \overline{T}} \max_{\lambda} \quad (A\,d + C\,\theta)^{\mathrm{T}}\,\lambda \tag{5a}$$

$$\text{s.t.} \quad e^{\mathrm{T}}\lambda = 1 \tag{5b}$$

$$-\,B^{\mathrm{T}}\lambda = 0 \tag{5c}$$

$$\lambda \in \mathbb{R}_{+}^{m}, \tag{5d}$$

which is equivalent to Problem (FT) since the optimal solution is guaranteed to lie at one of the vertices of T. The inner and outer maximization problems can be merged in order to achieve a single-level problem. We can then rewrite the objective function as follows:

$$(A\,d + C\,\theta)^{\mathrm{T}}\,\lambda = d^{\mathrm{T}}A^{\mathrm{T}}\lambda + \theta^{\mathrm{T}}C^{\mathrm{T}}\lambda \tag{6a}$$

$$= d^{\mathrm{T}}A^{\mathrm{T}}\lambda + \left[\theta^{\mathrm{N}} + \mathrm{diag}(x)\Delta\theta^{+} - (I - \mathrm{diag}(x))\Delta\theta^{-}\right]^{\mathrm{T}} C^{\mathrm{T}}\lambda \tag{6b}$$

$$= d^{\mathrm{T}} A^{\mathrm{T}} \lambda + \sum_{j \in J} c_j \left[\theta^{\mathrm{N}} + \operatorname{diag}(x) \Delta\theta^{+} - (I - \operatorname{diag}(x)) \Delta\theta^{-}\right] \lambda_j \quad (6c)$$

$$= d^{\mathrm{T}} A^{\mathrm{T}} \lambda + \sum_{j \in J} \sum_{i \in \Theta} c_{ji} \left[\lambda_j \left(\theta_i^{\mathrm{N}} - \Delta\theta_i^{-}\right) + \lambda_j \, x_i \left(\Delta\theta_i^{+} + \Delta\theta_i^{-}\right)\right] \quad (6d)$$

where I is the identity matrix of appropriate dimensionality and $\operatorname{diag}(\cdot)$ denotes a diagonal matrix. Note that C is an $m \times n_\theta$ matrix, and while c_j denotes the jth row vector of C, c_{ji} is the element at the jth row and ith column of C.

The objective function now contains the bilinear terms $\lambda_j \, x_i$. This bilinearity can be eliminated by applying exact linearization to the bilinear terms. By doing so, we obtain the following MILP reformulation of the flexibility test problem:

$$\begin{aligned}
\chi(d) = \max_{\lambda, \bar{\lambda}, x} \quad & d^{\mathrm{T}} A^{\mathrm{T}} \lambda + \sum_{j \in J} \sum_{i \in \Theta} c_{ji} \left[\lambda_j \left(\theta_i^{\mathrm{N}} - \Delta\theta_i^{-}\right) + \bar{\lambda}_{ij} \left(\Delta\theta_i^{+} + \Delta\theta_i^{-}\right)\right] \\
\text{s.t.} \quad & e^{\mathrm{T}} \lambda = 1 \\
& -B^{\mathrm{T}} \lambda = 0 \\
& \bar{\lambda}_{ij} \geq (\lambda_j - 1) + x_i \quad \forall\, i \in \Theta,\, j \in J \qquad \qquad (\mathrm{FT_{DFA}}) \\
& \bar{\lambda}_{ij} \leq \lambda_j \quad \forall\, i \in \Theta,\, j \in J \\
& \bar{\lambda}_{ij} \leq x_i \quad \forall\, i \in \Theta,\, j \in J \\
& \lambda \in \mathbb{R}_{+}^{m},\, \bar{\lambda} \in \mathbb{R}_{+}^{n_\theta \times m},\, x \in \{0,1\}^{n_\theta},
\end{aligned}$$

which consists of $3\, m\, n_\theta + n_z + 1$ constraints, $m(n_\theta + 1)$ continuous variables, and n_θ binary variables.

Affinely Adjustable Robust Optimization

In the following, we derive the affinely adjustable robust optimization (AARO) formulation for the flexibility test problem, and show its relationship to the flexibility analysis approach. In particular, we show that the AARO approach can be overly conservative, i.e. the obtained flexibility function value may be positive although z can be adjusted such that the design is feasible for all $\theta \in T$.

Following a general adjustable robust optimization approach,[11] the flexibility test problem can be formulated as follows:

$$\chi(d) = \min_{z(\theta), u \in \mathbb{R}} \quad u \tag{7a}$$

$$\text{s.t.} \quad A\, d + B\, z(\theta) + C\, \theta \leq u\, e \quad \forall\, \theta \in T, \tag{7b}$$

where z is expressed as a function of θ since it can be seen as the vector of recourse variables that are chosen after the realization of the uncertainty. Eq. (7b) states that all constraints have to be satisfied for every possible realization of the uncertainty, i.e. for all $\theta \in T$.

To show the connection with flexibility analysis, we write Problem (7) equivalently as

$$\chi(d) = \min_{z(\theta)} \max_{\theta \in T} \max_{j \in J} f_j(d, z(\theta), \theta). \tag{8}$$

The control function $z(\theta)$ itself has to be prespecified and cannot be changed later on, which is why it is a decision made in the outer minimization problem. Problem (8) is equivalent to Problem (FT) if $z(\theta)$ is chosen such that it is the optimal solution of Problem (FF) for every $\theta \in T$.

Applying Affine Control Functions

Problem (7) is a semi-infinite program since the number of possible control functions and the number of possible realizations of the uncertainty are both infinite. In order to derive a computationally tractable model that still guarantees feasibility for all $\theta \in T$, we restrict the set of control functions that can be selected. In static robust optimization, z has to be a constant, which means that no recourse is allowed. In AARO, z is expressed as an affine function of θ, i.e. $z(\theta) = p + Q\,\theta$, allowing recourse to a certain extent. Then, instead of z, p and Q become variables in the formulation. As we will show, it is still a restriction; however, this is a major improvement compared to the case without any recourse, and as it turns out, this linear approximation of recourse can often achieve the same level of flexibility. Substituting the affine function of θ for $z(\theta)$, the restricted flexibility test problem can be formulated as:

$$\bar{\chi}(d) = \min_{p \in \mathbb{R}^{n_z},\, Q \in \mathbb{R}^{n_z \times n_\theta}} \max_{\theta \in T} \max_{j \in J} \quad f_j(d, p, Q, \theta) \tag{9a}$$

$$= \min_{p \in \mathbb{R}^{n_z},\, Q \in \mathbb{R}^{n_z \times n_\theta}} \max_{\theta \in T} \min_{u \in \mathbb{R}} \quad u \tag{9b}$$

$$\text{s.t.} \quad A\,d + B\,(p + Q\,\theta) + C\,\theta \leq u\,e, \tag{9c}$$

for which we can show the following property:

Proposition 2. *Problem (9) has its optimal solution at a vertex of T.*

Proof. Problem (9) can be equivalently written as:

$$\bar{\chi}(d) = \min_{p \in \mathbb{R}^{n_z},\, Q \in \mathbb{R}^{n_z \times n_\theta}} \max_{\theta \in T} \min_{z,u} \quad u \tag{10a}$$

$$\text{s.t.} \quad A\,d + B\,z + C\,\theta \le u\,e \tag{10b}$$

$$z - (p + Q\,\theta) \le 0 \tag{10c}$$

$$-\,z + (p + Q\,\theta) \le 0 \tag{10d}$$

$$z \in \mathbb{R}^{n_z},\ u \in \mathbb{R}, \tag{10e}$$

where the affine control function has been incorporated by adding the two inequality constraints (10c) and (10d). For any fixed p and Q, the constraint functions are jointly convex in z and θ. Therefore, according to Theorem 1, the solution lies at a vertex of T for any p and Q. In particular, this holds true for the p and Q that minimize the objective function. Hence, Problem (10) has its optimal solution at a vertex of T, which is equivalently true for Problem (9). □

Proposition 2 implies that we only need to consider the vertices of T, of which there are finitely many. This allows us to obtain $\bar{\chi}(d)$ by solving:

$$\begin{aligned} \bar{\chi}(d) = \min_{p,Q,u} \quad & u \\ \text{s.t.} \quad & A\,d + B\,(p + Q\,\theta) + C\,\hat{\theta}_t \le u\,e \quad \forall\, t \in \overline{T} \\ & p \in \mathbb{R}^{n_z},\ Q \in \mathbb{R}^{n_z \times n_\theta},\ u \in \mathbb{R}, \end{aligned} \tag{$\text{FT}_{\overline{\text{AARO}}}$}$$

where $\overline{T}$ is the set of vertices of T.

Proposition 3. *Let $\chi(d)$ and $\bar{\chi}(d)$ be the flexibility function values obtained from solving Problems (FT_{TFA}) (or alternatively (FT_{DFA})) and ($\text{FT}_{\overline{\text{AARO}}}$), respectively. Then, $\chi(d) \le \bar{\chi}(d)$.*

Proof. Solving Problem ($\text{FT}_{\overline{\text{AARO}}}$) is equivalent to solving Problem (FT_{TFA})

with the additional constraint $z = p + Q\,\theta$ where $p \in \mathbb{R}^{n_z}$, $Q \in \mathbb{R}^{n_z \times n_\theta}$. Hence, ($\mathrm{FT}_{\overline{\mathrm{AARO}}}$) is a restriction of ($\mathrm{FT}_{\mathrm{TFA}}$), from which it follows that $\chi(d) \leq \bar{\chi}(d)$. □

Proposition 4. *For $n_\theta = 1$, $\chi(d) = \bar{\chi}(d)$.*

Proof. Let z^1 and z^2 be the solutions of Problem (FF) for $\theta = \theta^{\mathrm{L}}$ and $\theta = \theta^{\mathrm{U}}$, respectively. According to Theorem 1, $\chi(d)$ will be obtained at one of these two vertex solutions. By formulating the affine control function

$$z = \left[z^1 - \frac{(z^2 - z^1)}{\theta^{\mathrm{U}} - \theta^{\mathrm{L}}} \right] + \left(\frac{z^2 - z^1}{\theta^{\mathrm{U}} - \theta^{\mathrm{L}}} \right) \theta, \tag{11}$$

which corresponds to a line in the $(1 + n_z)$-dimensional (θ, z)-space, both vertex solutions can be considered. This implies that when solving Problem ($\mathrm{FT}_{\overline{\mathrm{AARO}}}$), the same controls ($z^1$ and z^2) can be applied at the vertices of T. According to Proposition 2, $\bar{\chi}(d)$ will be obtained at one of these two vertex solutions. Hence, $\chi(d) = \bar{\chi}(d)$. □

Following a similar argument, one arrives at a more general statement:

Proposition 5. *If the uncertainty set T is a polytope with $n_\theta + 1$ vertices, then $\chi(d) = \bar{\chi}(d)$.*

Proof. Suppose $z^1, z^2, \ldots, z^{n_\theta+1}$ are the solutions of Problem (FF) at the $n_\theta + 1$ vertices of T. All $n_\theta + 1$ vertex solutions can be expressed through an affine control function in the form of $z = p + Q\,\theta$, which represents an n_θ-dimensional hyperplane in the $(n_\theta + n_z)$-dimensional (θ, z)-space. Thus, the same solution will be obtained by solving Problems ($\mathrm{FT}_{\mathrm{TFA}}$) and ($\mathrm{FT}_{\overline{\mathrm{AARO}}}$). Hence, $\chi(d) =$

$\bar{\chi}(d)$. □

However, since uncertainty sets in the flexibility analysis problems are hyperboxes, Proposition 5 does not apply except in the case of $n_\theta = 1$. For $n_\theta \geq 2$, the number of vertices of the box uncertainty set is greater than $n_\theta + 1$. Then, we may encounter the situation in which not all vertex solutions of the original flexibility test problem can be expressed by an affine control function. In that case, the restricted flexibility test formulation (9) may fail in obtaining the same optimal solution. To formalize this intuitive result, we state the following:

Proposition 6. *For $n_\theta \geq 2$, there exist constraint matrices A, B, C, and designs d such that $\chi(d) < \bar{\chi}(d)$.*

Proof. We prove this proposition by finding an example for $n_\theta = 2$ in which $\chi(d) < \bar{\chi}(d)$. The same result then follows for $n_\theta > 2$ since the case of $n_\theta = 2$ can be seen as a special case of $n_\theta > 2$.

Consider the example with the following four constraints:

$$f_1 = -z \leq 0 \tag{12a}$$

$$f_2 = z - \theta_2 \leq 0 \tag{12b}$$

$$f_3 = z - \theta_1 \leq 0 \tag{12c}$$

$$f_4 = -20 - z + \theta_1 + \theta_2 \leq 0 \tag{12d}$$

which form the polytope that is shown in Figure 3. The uncertainty set is chosen to be $T = \{(\theta_1, \theta_2) : 0 \leq \theta_1 \leq 20,\ 0 \leq \theta_2 \leq 20\}$.

By solving Problem ($\mathrm{FT_{DFA}}$) for this example, we obtain $\chi = 0$. However,

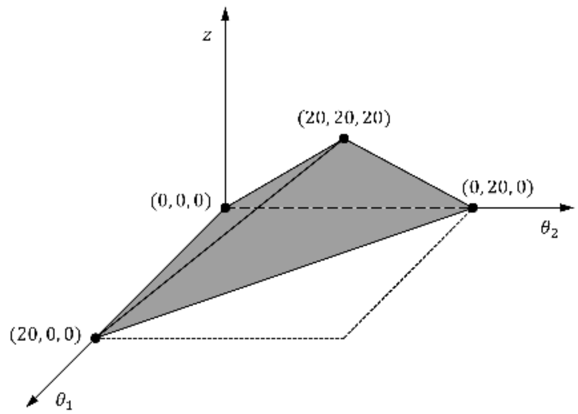


Figure 3: Illustrative example with $n_\theta = 2$, where $\chi(d) < \bar{\chi}(d)$.

$\bar{\chi} = 5$ is obtained by solving Problem ($\text{FT}_{\overline{\text{AARO}}}$). Thus, in this particular case with $n_\theta = 2$, we have $\chi < \bar{\chi}$, which proves the proposition. □

In Figure 3, one can see that for each of the vertices of T, there is exactly one feasible z. A plane in the 3-dimensional (θ, z)-space, which could be described by an affine control function, can cover at most three of the four vertex solutions. Therefore, while the process is feasible for the entire uncertainty set if z can be freely adjusted within the feasible region, this cannot be achieved if z is restricted to be an affine function of θ.

Another geometric interpretation of Proposition 6 can be obtained by examining the projection of the feasible region onto the θ-space. In our example, as one can see in Figure 3, the projection of the 3-dimensional polytope representing the feasible region onto the 2-dimensional θ-space covers exactly T; thus, $\chi = 0$. However, one cannot find a plane such that the projection of the intersection between the plane and the polytope covers T; hence, $\bar{\chi} > 0$.

Formulating Robust Counterpart

If T has a large number of vertices, Problem ($\text{FT}_{\overline{\text{AARO}}}$) can quickly become computationally intractable. In order to avoid enumerating all vertices, we first notice that the restricted flexibility test problem given by Eq. (9a) can be equivalently written as follows by interchanging the two inner maximizations:

$$\bar{\chi}(d) = \min_{p \in \mathbb{R}^{n_z},\, Q \in \mathbb{R}^{n_z \times n_\theta}} \max_{j \in J} \max_{\theta \in T} f_j(d, p, Q, \theta), \tag{13}$$

from which it follows that we arrive at the same solution by applying a constraint-wise worst-case approach, i.e. by taking $\max_{\theta \in T} f_j$ for each individual $j \in J$. Hence, the restricted flexibility test problem can be reformulated as follows:

$$\bar{\chi}(d) = \min_{p,Q,u} \quad u \tag{14a}$$

$$\text{s.t.} \quad a_j\, d + b_j\, p + \max_{\theta \in T} \{ (b_j\, Q + c_j)\, \theta \} \le u \quad \forall\, j \in J \tag{14b}$$

$$p \in \mathbb{R}^{n_z},\, Q \in \mathbb{R}^{n_z \times n_\theta},\, u \in \mathbb{R}. \tag{14c}$$

Problem (14) is a bilevel problem with m lower-level problems. For each j, the corresponding lower-level problem is:

$$\max_{\theta} \quad (b_j\, Q + c_j)\, \theta \tag{15a}$$

$$\text{s.t.} \quad \theta^{\text{L}} \le \theta \le \theta^{\text{U}}, \tag{15b}$$

of which the dual is:

$$\min_{\mu_j,\nu_j} \quad \left(\theta^{\mathrm{U}}\right)^{\mathrm{T}} \mu_j - \left(\theta^{\mathrm{L}}\right)^{\mathrm{T}} \nu_j \tag{16a}$$

$$\text{s.t.} \quad \mu_j - \nu_j = \left(b_j\, Q + c_j\right)^{\mathrm{T}} \tag{16b}$$

$$\mu_j \in \mathbb{R}_+^{n_\theta},\ \nu_j \in \mathbb{R}_+^{n_\theta}. \tag{16c}$$

By substituting the dual formulations of the lower-level problems into Eq. (14), we obtain the following single-level problem, which is generally referred to as the affinely adjustable robust counterpart:[8]

$$\begin{aligned} \bar{\chi}(d) = \min_{p,Q,u,\mu,\nu} \quad & u \\ \text{s.t.} \quad & a_j\, d + b_j\, p + \left[\left(\theta^{\mathrm{U}}\right)^{\mathrm{T}} \mu_j - \left(\theta^{\mathrm{L}}\right)^{\mathrm{T}} \nu_j\right] \le u\, e \quad \forall\, j \in J \\ & \mu_j - \nu_j = \left(b_j\, Q + c_j\right)^{\mathrm{T}} \quad \forall\, j \in J \\ & p \in \mathbb{R}^{n_z},\ Q \in \mathbb{R}^{n_z \times n_\theta},\ u \in \mathbb{R},\ \mu \in \mathbb{R}_+^{n_\theta \times m},\ \nu \in \mathbb{R}_+^{n_\theta \times m}, \end{aligned} \tag{FT$_{\mathrm{AARO}}$}$$

which is an LP with $m(n_\theta + 1)$ constraints and $n_\theta(2m + n_z) + n_z + 1$ variables. Due to strong duality, Problems (14) and (FT$_{\mathrm{AARO}}$) have the same objective function value at the optimal solution.

Flexibility Index Problem

Problem Statement

Define the uncertainty set as $T(\delta) = \left\{\theta : \theta^{\mathrm{N}} - \delta\, \Delta\theta^- \le \theta \le \theta^{\mathrm{N}} + \delta\, \Delta\theta^+\right\}$, where δ is a nonnegative scalar, and $\Delta\theta^-$ and $\Delta\theta^+$ are incremental negative and positive deviations from the nominal value, respectively. The flexibility index problem[7] can then be stated as follows: For a given design d, find the largest δ such that by proper adjustment of the control variables z, the inequalities $f_j(d,z,\theta) \leq 0$, $j \in J$, hold for all $\theta \in T(\delta)$. This maximum δ is referred to as the flexibility index $F(d)$.

Traditional Flexibility Analysis

The flexibility index can be computed as follows:[7]

$$F(d) = \max_{\delta \in \mathbb{R}_+} \quad \delta \tag{17a}$$

$$\text{s.t.} \quad \max_{\theta \in T(\delta)} \min_{z \in \mathbb{R}^{n_z}} \max_{j \in J} f_j(d,z,\theta) \leq 0, \tag{17b}$$

which is equivalent to the minimum δ for which the feasibility function $\psi(d,\theta)$ is zero, i.e.

$$F(d) = \min_{\delta \in \mathbb{R}_+, \theta \in T(\delta)} \quad \delta \tag{18a}$$

$$\text{s.t.} \quad \psi(d,\theta) = 0. \tag{18b}$$

By applying the active-set method,[15] Problem (18) can be formulated as the following MILP:

$$
\begin{aligned}
F(d) = \min_{\theta,z,\lambda,s,y,\delta} \quad & \delta \\
\text{s.t.} \quad & A\,d + B\,z + C\,\theta + s = 0 \\
& e^{\mathrm{T}}\lambda = 1 \\
& B^{\mathrm{T}}\lambda = 0 \\
& \lambda \le y \\
& s \le M(e - y) \\
& e^{\mathrm{T}} y \le n_z + 1 \\
& \theta^{\mathrm{N}} - \delta\,\Delta\theta^{-} \le \theta \le \theta^{\mathrm{N}} + \delta\,\Delta\theta^{+} \\
& z \in \mathbb{R}^{n_z},\ \lambda \in \mathbb{R}^{m}_{+},\ s \in \mathbb{R}^{m}_{+},\ y \in \{0,1\}^{m},\ \delta \in \mathbb{R}_{+},
\end{aligned}
\tag{FI$_{\text{TFA}}$}
$$

which has the same numbers of constraints and variables as Problem (FT$_{\text{TFA}}$).

Duality-based Flexibility Analysis

Define $\theta = \theta^{\mathrm{N}} + \delta\,\tilde{\theta}$ with $\tilde{\theta} \in \widetilde{T}$, where

$$\widetilde{T} = \left\{\tilde{\theta} : \tilde{\theta}_i = x_i\,\Delta\theta_i^{+} - (1 - x_i)\Delta\theta_i^{-},\ x_i \in \{0,1\}\ \ \forall\, i \in \Theta\right\}. \tag{19}$$

The flexibility index problem can then be stated as:

$$F(d) = \min_{\tilde{\theta}\in\widetilde{T}(\delta)} \max_{z,\delta} \quad \delta \tag{20a}$$

$$\text{s.t.} \quad A\,d + B\,z + C\left(\theta^{\mathrm{N}} + \delta\,\tilde{\theta}\right) \le 0 \tag{20b}$$

$$z \in \mathbb{R}^{n_z},\ \delta \in \mathbb{R}_{+}, \tag{20c}$$

where the dual of the inner maximization problem for a given $\tilde{\theta}$ is:

$$\delta(d,\tilde{\theta}) = \min_{\lambda} \quad \left(-A\,d - C\,\theta^{\mathrm{N}}\right)^{\mathrm{T}} \lambda \tag{21a}$$

$$\text{s.t.} \quad B^{\mathrm{T}} \lambda = 0 \tag{21b}$$

$$\tilde{\theta}^{\mathrm{T}} C^{\mathrm{T}} \lambda \geq 1 \tag{21c}$$

$$\lambda \in \mathbb{R}^m_+. \tag{21d}$$

The flexibility index problem then becomes:

$$F(d) = \min_{\tilde{\theta},\lambda} \quad \left(-A\,d - C\,\theta^{\mathrm{N}}\right)^{\mathrm{T}} \lambda \tag{22a}$$

$$\text{s.t.} \quad B^{\mathrm{T}} \lambda = 0 \tag{22b}$$

$$\tilde{\theta}^{\mathrm{T}} C^{\mathrm{T}} \lambda \geq 1 \tag{22c}$$

$$\tilde{\theta} \in \widetilde{T},\ \lambda \in \mathbb{R}^m_+, \tag{22d}$$

which following a similar reasoning as in ($\mathrm{FT}_{\mathrm{DFA}}$) can be reformulated into:

$$\begin{aligned}
F(d) = \min_{\lambda,\bar{\lambda},x} \quad & \left(-A\,d - C\,\theta^{\mathrm{N}}\right)^{\mathrm{T}} \lambda \\
\text{s.t.} \quad & B^{\mathrm{T}} \lambda = 0 \\
& \sum_{j\in J} \sum_{i\in\Theta} c_{ji} \left[-\lambda_j \Delta\theta_i^- + \bar{\lambda}_{ij} \left(\Delta\theta_i^+ + \Delta\theta_i^-\right)\right] \geq 1 \\
& \bar{\lambda}_{ij} \geq (\lambda_j - 1) + x_i \quad \forall\, i \in \Theta,\ j \in J \\
& \bar{\lambda}_{ij} \leq \lambda_j \quad \forall\, i \in \Theta,\ j \in J \\
& \bar{\lambda}_{ij} \leq x_i \quad \forall\, i \in \Theta,\ j \in J \\
& \lambda \in \mathbb{R}^m_+,\ \bar{\lambda} \in \mathbb{R}^{n_\theta \times m}_+,\ x \in \{0,1\}^{n_\theta},
\end{aligned} \tag{$\mathrm{FI}_{\mathrm{DFA}}$}$$

which has the same numbers of constraints and variables as Problem ($\mathrm{FT}_{\mathrm{DFA}}$).

Affinely Adjustable Robust Optimization

If we follow a similar approach as in Section b to derive the AARO formulation, but directly apply the uncertainty set $T(\delta)$, we will arrive at a nonlinear formulation due to the dependence of the uncertainty set on δ, which is a decision variable. In order to avoid this nonlinearity, we define

$$\theta = \theta^{\mathrm{N}} - \delta\,\Delta\theta^{-} + w\,\delta(\Delta\theta^{-} + \Delta\theta^{+}) \tag{23}$$

where w is the vector of normalized uncertain parameters for which the uncertainty set can be written as

$$W = \{w : 0 \leq w \leq e,\, w \in \mathbb{R}^{n_\theta}\}\,. \tag{24}$$

Note that W is a fixed uncertainty set. We now choose the affine control function to be $z = p + Q\,w$, so the restricted flexibility index problem becomes:

$$\overline{F}(d) = \max_{p,Q,\delta} \quad \delta \tag{25a}$$

$$\text{s.t.} \quad a_j\,d + b_j\,p + c_j(\theta^{\mathrm{N}} - \delta\,\Delta\theta^{-})$$

$$+ \max_{w \in W} \{[b_j\,Q + c_j\,\delta(\Delta\theta^{-} + \Delta\theta^{+})]\,w\} \leq 0 \quad \forall\, j \in J \tag{25b}$$

$$p \in \mathbb{R}^{n_z},\, Q \in \mathbb{R}^{n_z \times n_\theta},\, \delta \in \mathbb{R}_{+}. \tag{25c}$$

The dual of the maximization problem in each constraint j is:

$$\min_{\mu_j} \quad e^{\mathrm{T}} \mu_j \tag{26a}$$

$$\text{s.t.} \quad \mu_j \geq \left[b_j Q + c_j \, \delta (\Delta\theta^- + \Delta\theta^+) \right]^{\mathrm{T}} \tag{26b}$$

$$\mu_j \in \mathbb{R}_+^{n_\theta}, \tag{26c}$$

which leads to the following affinely adjustable robust counterpart of the flexibility index problem:

$$\begin{aligned}
\overline{F}(d) = \max_{p,Q,\mu,\delta} \quad & \delta \\
\text{s.t.} \quad & a_j \, d + b_j \, p + c_j (\theta^{\mathrm{N}} - \delta \, \Delta\theta^-) + e^{\mathrm{T}} \mu_j \leq 0 \quad \forall \, j \in J \\
& \mu_j \geq \left[b_j Q + c_j \, \delta (\Delta\theta^- + \Delta\theta^+) \right]^{\mathrm{T}} \quad \forall \, j \in J \\
& p \in \mathbb{R}^{n_z}, \, Q \in \mathbb{R}^{n_z \times n_\theta}, \, \mu \in \mathbb{R}_+^{n_\theta \times m}, \, \delta \in \mathbb{R}_+,
\end{aligned} \tag{FI$_{\mathrm{AARO}}$}$$

which is an LP with $m(n_\theta + 1)$ constraints and $n_\theta(m + n_z) + n_z + 1$ variables.

Design Under Uncertainty with Flexibility Constraints

Problem Statement

The design under uncertainty problem with flexibility constraints[6] is formulated as follows:

$$\eta = \min_{d, \bar{z}} \quad \hat{c}^{\mathrm{T}} d + \sum_{s \in S} \varphi_s \, \bar{c}^{\mathrm{T}} \bar{z}_s \tag{27a}$$

$$\text{s.t.} \quad A \, d + B \, \bar{z}_s + C \, \bar{\theta}_s \leq 0 \quad \forall \, s \in S \tag{27b}$$

$$\max_{\theta \in T} \min_{z \in \mathrm{R}^{n_z}} \max_{j \in J} \{ a_j \, d + b_j \, z + c_j \, \theta \} \leq 0 \tag{27c}$$

$$d \in \mathbb{R}^{n_d},\ \bar{z} \in \mathbb{R}^{n_z \times h}, \tag{27d}$$

where $\hat{c}$ and $\bar{c}$ are vectors of cost coefficients. The objective function is an approximation of the total expected cost, which consists of two parts: the capital cost associated with the design, $\hat{c}^{\mathrm{T}} d$, and a scenario-based approximation of the expected operating cost, $\sum_{s \in S} \varphi_s\, \bar{c}^{\mathrm{T}} \bar{z}_s$. In the scenario set $S = \{1, 2, \ldots, h\}$, each scenario is denoted by the index s and is characterized by $\bar{\theta}_s$, the value that the uncertain parameter θ takes in this particular scenario, and the corresponding probability φ_s, for which $\sum_{s \in S} \varphi_s = 1$. For each scenario, a different control, $\bar{z}_s$, is determined, which satisfies Eq. (27b). The expected operating cost is approximated by calculating the sum of the operating costs for the h representative scenarios in S, each weighted with the corresponding probability.

In addition to Eq. (27b), which ensures that the design is feasible for all preselected scenarios, the flexibility constraints given by Eq. (27c) further guarantee feasibility for all $\theta \in T$ given that the control variable z can be adjusted depending on the realization of the uncertain parameter.

Flexibility Analysis

Halemane and Grossmann[6] solve Problem (27) with an iterative column-and-constraint generation approach. The algorithm relies on the fact that a design is feasible for all $\theta \in T$ if it is feasible for the worst-case realization of the uncertainty, which lies at one of the vertices of T. In each iteration, a relaxation of Problem (27) is solved, where Eq. (27c) is replaced by a set of constraints of the form $f_j(d, \hat{z}_t, \hat{\theta}_t)\ \forall\, j \in J$, where $\hat{\theta}_t$ is a vertex of T. Then, a flexibility test is performed for the obtained design. If the design is feasible, the algorithm terminates; otherwise, the critical point (another vertex) obtained from the flexibility test is added to the formulation, which is solved in the next iteration to determine the next design suggestion. The complete algorithm is as follows:

Step 1 Set $k = 0$. Choose an initial set $\widehat{T}_0$ consisting of N_0 critical points.

Step 2 Solve the following problem:

$$\min_{d,\bar{z},\hat{z}} \quad \hat{c}^{\mathrm{T}} d + \sum_{s \in S} \varphi_s \, \bar{c}^{\mathrm{T}} \bar{z}_s \tag{28a}$$

$$\text{s.t.} \quad A\, d + B\, \bar{z}_s + C\, \bar{\theta}_s \leq 0 \quad \forall\, s \in S \tag{28b}$$

$$A\, d + B\, \hat{z}_t + C\, \hat{\theta}_t \leq 0 \quad \forall\, t \in \widehat{T}_k \tag{28c}$$

$$d \in \mathbb{R}^{n_d},\ \bar{z} \in \mathbb{R}^{n_z \times h},\ \hat{z} \in \mathbb{R}^{n \times N_k} \tag{28d}$$

to obtain design d_k.

Step 3 Solve Problem ($\mathrm{FT}_{\mathrm{TFA}}$) or ($\mathrm{FT}_{\mathrm{DFA}}$) by setting $d = d_k$, and obtain critical point θ_k^c. If $\chi(d_k) \leq 0$, stop; otherwise, go to Step 4.

Step 4 Set $\hat{\theta}_{k+1} = \theta_k^c$, $N_{k+1} = N_k + 1$, and define $\widehat{T}_{k+1} = \{1, 2, \ldots, N_{k+1}\}$. Set $k = k + 1$ and go to Step 2.

The algorithm converges in a finite number of iterations since there is a finite number of vertices. Note that the only difference between the traditional and the duality-based flexibility analysis approaches is the flexibility test problem that is solved in Step 3.

There are different approaches for choosing the initial set of critical points $\widehat{T}_0$. For example, one effective strategy[1] is to determine the critical points for each constraint by examining the signs of the coefficients in matrix C and use these points as the initial set. For the remainder of the paper, we refer to the variant of the algorithm applying this initialization strategy as $\mathrm{DF}^*_{\mathrm{TFA}}$ or $\mathrm{DF}^*_{\mathrm{DFA}}$ (depending on whether the TFA or DFA flexibility test problem is solved). Alternatively, one could also simply let $\widehat{T}_0$ be empty; this variant of the algorithm will be denoted by $\mathrm{DF}^0_{\mathrm{TFA}}$ or $\mathrm{DF}^0_{\mathrm{DFA}}$.

It is worth mentioning that very recently, similar column-and-constraint generation algorithms have been proposed to solve the two-stage robust optimization problem that allows full adjustability in the recourse.[43,44] This is just another indicator for the strong connection between flexibility analysis and robust optimization, and example of the pioneering work in flexibility analysis that has long preceded the era of robust optimization.

Affinely Adjustable Robust Optimization

Unlike the flexibility analysis approach, the AARO approach does not require an iterative framework. Here, we only need to solve a single LP. In order to obtain the AARO formulation, we simply take Problem ($\mathrm{FT}_{\mathrm{AARO}}$), set $u = 0$ to ensure feasibility, and add Eqs. (27a) and (27b) to describe the objective function. Hence, we arrive at the following formulation:

$$
\begin{aligned}
\eta = \min_{d,\bar{z},p,Q,\mu,\nu} \quad & \hat{c}^{\mathrm{T}} d + \sum_{s \in S} \varphi_s \, \bar{c}^{\mathrm{T}} \bar{z}_s \\
\text{s.t.} \quad & A\, d + B\, \bar{z}_s + C\, \bar{\theta}_s \leq 0 \quad \forall\, s \in S \\
& a_j\, d + b_j\, p + \left[\left(\theta^{\mathrm{U}}\right)^{\mathrm{T}} \mu_j - \left(\theta^{\mathrm{L}}\right)^{\mathrm{T}} \nu_j \right] \leq 0 \quad \forall\, j \in J \\
& \mu_j - \nu_j = \left(b_j\, Q + c_j\right)^{\mathrm{T}} \quad \forall\, j \in J \\
& d \in \mathbb{R}^{n_d},\ \bar{z} \in \mathbb{R}^{n_z \times h},\ p \in \mathbb{R}^{n_z},\ Q \in \mathbb{R}^{n_z \times n_\theta},\ \mu \in \mathbb{R}_{+}^{n_\theta \times m},\ \nu \in \mathbb{R}_{+}^{n_\theta \times m}.
\end{aligned}
\tag{DF$_{\mathrm{AARO}}$}
$$

Note that in Problem (DF$_{\mathrm{AARO}}$), the control variables for the scenarios used to compute the expected cost and the ones used to guarantee feasibility for all $\theta \in T$ are treated differently. While $\bar{z}_s$ are fully adjustable, the adjustable controls in the flexibility constraints are restricted to affine functions.

For the sake of comparison, we also present a formulation in which $\bar{z}_s$ are set according to the same affine functions:

$$
\begin{aligned}
\eta' = \min_{d,p,Q,\mu,\nu} \quad & \hat{c}^{\mathrm{T}} d + \sum_{s \in S} \varphi_s \, \bar{c}^{\mathrm{T}} \left(p + Q\, \bar{\theta}_s\right) \\
\text{s.t.} \quad & A\, d + B\, \left(p + Q\, \bar{\theta}_s\right) + C\, \bar{\theta}_s \leq 0 \quad \forall\, s \in S \\
& a_j\, d + b_j\, p + \left[\left(\theta^{\mathrm{U}}\right)^{\mathrm{T}} \mu_j - \left(\theta^{\mathrm{L}}\right)^{\mathrm{T}} \nu_j \right] \leq 0 \quad \forall\, j \in J \\
& \mu_j - \nu_j = \left(b_j\, Q + c_j\right)^{\mathrm{T}} \quad \forall\, j \in J \\
& d \in \mathbb{R}^{n_d},\ p \in \mathbb{R}^{n_z},\ Q \in \mathbb{R}^{n_z \times n_\theta},\ \mu \in \mathbb{R}_{+}^{n_\theta \times m},\ \nu \in \mathbb{R}_{+}^{n_\theta \times m}.
\end{aligned}
\tag{DF$'_{\mathrm{AARO}}$}
$$

Let η and η' be the total expected costs at the optimal solutions of Problems (DF$_{\mathrm{AARO}}$) and (DF$'_{\mathrm{AARO}}$), respectively. Clearly, since Problem (DF$'_{\mathrm{AARO}}$) is a restriction of Problem (DF_{AARO}), $\eta \leq \eta'$. The advantage of Problem (DF'_{AARO}) is that it does not involve the variables $\bar{z}_s$, which, however, usually does not translate into significant reductions in computational times.

Numerical Examples

In the following, we apply the proposed models to flexibility analysis problems for three different examples. While the first two examples are meant to be illustrative, the third one is significantly larger in size and allows more insights into the computational performance of the different approaches. All models were implemented in GAMS 24.4.1,[70] and the commercial solver CPLEX 12.6.1 was applied to solve the LPs and MILPs on an Intel® Core™ i7-2600 machine at 3.40 GHz with 8 hardware threads and 8 GB RAM running Windows 7 Professional. Unless specified otherwise, the LPs were solved with the concurrent option using all 8 threads. Similarly, MILPs were also solved in parallel using all available threads.

Example 1: Heat Exchanger Network

This first example of a small heat exchanger network (HEN) is based on an example introduced by Grossmann and Floudas.[15] The HEN consisting of two hot streams, two cold streams, three heat exchangers and one cooler is shown in Figure 4. Here, the uncertainty lies in the inlet temperatures of the hot and cold streams; hence, the four uncertain parameters are T_1, T_3, T_5, and T_8. The nominal values for the uncertain temperatures are shown in Figure 4, and the maximum deviations from the nominal values for each temperature are assumed to be ±5 K. The control variable is the heat load in the cooler denoted by Q_C. We consider as design variable $T_7^{\max}$, which is the upper bound on T_7.

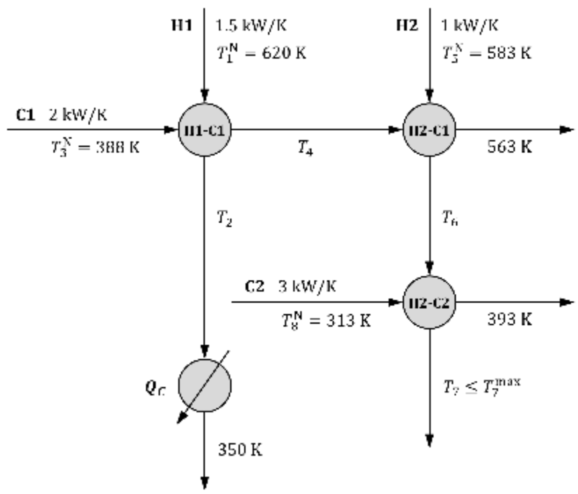


Figure 4: Example 1, HEN with four uncertain inlet temperatures and one control variable (Q_C).

The five inequality constraints for the given HEN are the following:

$$-350 - 0.67\,Q_C + T_3 \le 0 \tag{29a}$$

$$1388.5 + 0.5\,Q_C - 0.75\,T_1 - T_3 - T_5 \le 0 \tag{29b}$$

$$2044 + Q_C - 1.5\,T_1 - 2\,T_3 - T_5 \le 0 \tag{29c}$$

$$2830 + Q_C - 1.5\,T_1 - 2\,T_3 - T_5 - 2\,T_8 \le 0 \tag{29d}$$

$$-2830 - T_7^{\max} - Q_C + 1.5\,T_1 + 2\,T_3 + T_5 + T_8 \le 0 \tag{29e}$$

For the initial design with $T_7^{\max} = 317$ K, we solve the flexibility test and flexibility index problems by applying the proposed models from the TFA, DFA, and AARO approaches. The results are shown in Tables 1 and 2. Notice that all three approaches obtain the same results, which implies that in this case, the same level of flexibility can be achieved by restricting the control variable to take the form of an affine function of the uncertain parameters. Tables 1 and 2 also show the numbers of constraints, continuous, and binary variables in each model, which indicate the small size of this problem. As a result, the solution times are marginal.

Table 1: Flexibility test results for Example 1.

Model	$\chi(d), \bar{\chi}(d)$	# of Constraints	# of Cont. Variables	# of Bin. Variables	Solution Time [s]
(FT_{TFA})	2.0	26	16	5	0.11
(FT_{DFA})	2.0	62	25	4	0.06
(FT_{AARO})	2.0	25	46		0.05

Table 2: Flexibility index results for Example 1.

Model	$F(d), \overline{F}(d)$	# of Constraints	# of Cont. Variables	# of Bin. Variables	Solution Time [s]
(FI_{TFA})	0.7	26	16	5	0.06
(FI_{DFA})	0.7	62	25	4	0.05
(FI_{AARO})	0.7	25	26		0.03

Now we optimize the design while satisfying the flexibility constraints. The cost coefficients for the design variable $T_7^{\max}$ and the control variable Q_C are set to 2 and 1, respectively. For the approximation of the expected operating cost, three scenarios are considered for which the data are shown in Table 3. Note that Scenario 2 is the nominal case.

Table 3: Data for discrete scenarios considered in Example 1.

Scenario	T_1	T_3	T_5	T_8	φ
1	615	383	578	308	0.25
2	620	388	583	313	0.50
3	625	393	588	318	0.25

Table 4 shows the results for the design under uncertainty problem. Recall that in the case of the iterative algorithms, superscript 0 denotes the variants in which the initial set of critical points $\widehat{T}_0$ is empty, while superscript * denotes the initialization strategy in which a critical point is included in $\widehat{T}_0$ for each constraint. The numbers of constraints and variables refer to the LP that is solved to obtain the optimal design; in the TFA and DFA approaches, this is the LP solved in the final iteration of the algorithm. Here, one observes the trade-off between the number of iterations and the sizes of the LPs solved at each iteration. In DF^0_{TFA} and DF^0_{DFA}, only one critical point needs to be considered, resulting in two small LPs solved in two iterations. DF^*_{TFA} and DF^*_{DFA} create a larger initial set of critical points, which leads to a larger LP; however, now only one iteration is required. Since a flexibility test has to be performed at each iteration in addition to solving the LP, reducing in the number of iterations can be of great computational benefit. In this particular case, the smaller number of iterations leads to shorter solution times.

By solving Problem (DF_{AARO}), we immediately arrive at the optimal solution. No iterations are required and no additional flexibility test needs to be performed; hence, although the LP to be solved is larger, the solution time is significantly less than the ones required by the TFA and DFA algorithms. Furthermore, one can see the difference between Problems (DF_{AARO}) and (DF'_{AARO}),

Table 4: Design under uncertainty results for Example 1.

Model/ Algorithm	Expected Cost	# of Iterations	# of Constraints	# of Cont. Variables	Solution Time [s]
$\mathrm{DF}^0_{\mathrm{TFA}}$	724	2	20	5	0.47
$\mathrm{DF}^*_{\mathrm{TFA}}$	724	1	30	7	0.23
$\mathrm{DF}^0_{\mathrm{DFA}}$	724	2	20	5	0.49
$\mathrm{DF}^*_{\mathrm{DFA}}$	724	1	30	7	0.24
($\mathrm{DF}_{\mathrm{AARO}}$)	724		40	49	0.10
($\mathrm{DF'}_{\mathrm{AARO}}$)	727		40	46	0.09

where the latter leads to a slightly higher total expected cost due to the restriction of the control variable to an affine function also in the three scenarios used to compute the expected cost.

Example 2: Process Flowsheet

Consider the simple process flowsheet shown in Figure 5. In this process, Material A is fed into a reactor where it reacts to Materials B and C at a fixed conversion ratio ξ. Materials B and C are then separated in an ideal separator in order to satisfy product demands D_B and D_C. Here, the uncertainty lies in the demands and in the effective geometries of the inlet pipe and of the reactor, which have an impact on the flow capacities in the pipe and the reactor. The geometric properties of the pipe and the reactor are represented by the characteristic numbers R and V, respectively; these parameters may be uncertain due to fouling or wear and tear. The control variable here is the feed flowrate m_A.

The given process is represented by the following inequality constraints:

$$-m_A + 0.2\,V \leq 0 \tag{30a}$$

$$m_A - V \leq 0 \tag{30b}$$

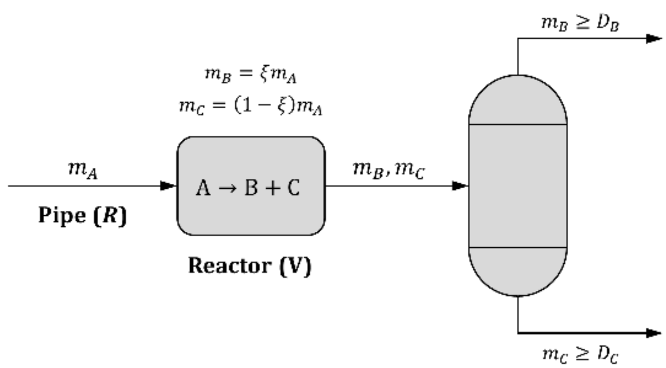


Figure 5: Example 2, simple process with uncertainty in product demands and equipment geometries.

$$m_A - R \leq 0 \tag{30c}$$

$$-30 - m_A + 0.8\,V + 1.2\,R \leq 0 \tag{30d}$$

$$-\xi\, m_A + D_B \leq 0 \tag{30e}$$

$$-(1-\xi)m_A + D_C \leq 0 \tag{30f}$$

where Eq. (30a) states that the reactor requires a minimum flowrate depending on its size, which at the same time imposes an upper bound on the flowrate as expressed in Eq. (30b). Similarly, the flowrate is limited by the size of the pipe, which is stated in Eq. (30c). The critical constraint is Eq. (30d). Here, we assume that some flow conditions, such as turbulent flow, have to be satisfied in the reactor in order for the reaction to be effective. The required flowrate depends on both the pipe and the reactor geometries; the correlation for this relationship is approximated by the linear function in Eq. (30d). Finally, Eqs. (30e) and (30f) state that the product flowrates have to be greater than or equal to the demands.

We solve the flexibility test and flexibility index problems for $\xi = 0.6$ and the following uncertainty sets: $D_B \in [6, 8]$, $D_C \in [3, 5]$, $R \in [15, 25]$, and $V \in [14, 26]$. In the nominal case, each uncertain parameter takes the value of the midpoint in the corresponding uncertainty range. The results are shown in Table 5. One can see that the flexibility analysis and AARO approaches obtain different solutions, namely $\chi(d) < \bar{\chi}(d)$ and $F(d) > \overline{F}(d)$, which is due to the restriction of the control variable to affine functions in the AARO models. In this case, the TFA and DFA models correctly report that the process is feasible for every possible realization of the uncertainty given that the feed flowrate can be properly adjusted, while the AARO model fails to do so. Note that we do not report computational results due to the small problem sizes and marginal solution times as was the case in Example 1.

Table 5: Flexibility test and flexibility index results for Example 2.

Approach	$\chi(d), \bar{\chi}(d)$	$F(d), \overline{F}(d)$
TFA/DFA	−0.25	1.09
AARO	1.10	0.78

Example 3: Planning of Large-Scale Process Network

In this example, we consider the long-term production planning of a large-scale process network representing a petrochemical complex.[71] The given process network, which is schematically shown in Figure 6, consists of 38 processes and 28 chemicals. The planning model is shown in the following. Note that the nomenclature for this model is independent from and therefore not to be confused with the one used for the models presented in the previous sections.

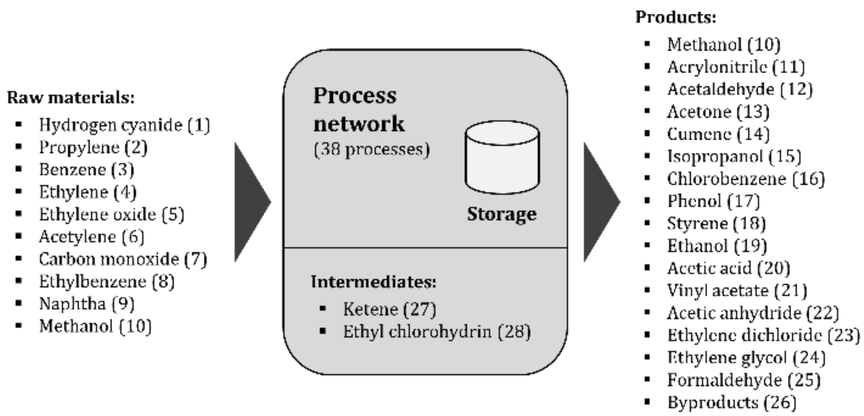


Figure 6: Schematic of the petrochemical complex considered in Example 3 (figure adapted from Park et al.[72]). For the detailed process network, see the original paper by Sahinidis et al.[71]

The model formulation consists of the following constraints:

$$Q_j^0 + \sum_{t'=1}^{t} \left(\sum_{i \in \hat{I}_j} \mu_{ij} P_{it'} - \sum_{i \in \bar{I}_j} \mu_{ij} P_{it'} + W_{jt'} - D_{jt'} \right) \geq Q_j^{\min} \quad \forall\, j \in J,\, t \in T \tag{31a}$$

$$Q_j^0 + \sum_{t'=1}^{t} \left(\sum_{i \in \hat{I}_j} \mu_{ij} P_{it'} - \sum_{i \in \bar{I}_j} \mu_{ij} P_{it'} + W_{jt'} - D_{jt'} \right) \leq Q_j^{\max} \quad \forall\, j \in J,\, t \in T \tag{31b}$$

$$P_{it} \leq P_i^{\max} \quad \forall\, i \in I,\, t \in T \tag{31c}$$

$$W_{jt} \leq W_{jt}^{\max} - \sum_{j' \in \bar{J}_j} \xi_{jj'} D_{j't} \quad \forall\, j \in J,\, t \in T \tag{31d}$$

$$P_{it} \geq 0 \quad \forall\, i \in I,\, t \in T \tag{31e}$$

$$W_{jt} \geq 0 \quad \forall\, j \in J,\, t \in T \tag{31f}$$

where J, I, and T are the sets of chemicals, processes, and time periods, respectively. Q_j^0 is the initial inventory of chemical j, and $Q_j^{\min}$ and $Q_j^{\max}$ are the minimum and maximum inventory levels, respectively. P_{it} denotes the amount of main product produced by process i in time period t. The production or consumption of chemical j by process i is given by a conversion factor, denoted by μ_{ij}, with respect to the main product; hence, $\mu_{ij} P_{it}$ is the amount of chemical j that is produced or consumed by process i in time period t. The sets of processes producing and consuming chemical j are denoted by $\hat{I}_j$ and $\bar{I}_j$, respectively. W_{jt} denotes the amount of chemical j purchased, and D_{jt} is the demand for chemical j in time period t.

Eqs. (31a) and (31b) are the inventory constraints, which ensure that the inventory level is within the given bounds at any time. Eq. (31c) sets the production capacity for each process. In Eq. (31d), the assumption is that the purchase limit for chemical j depends on the demand for products that require chemical j as feed, which is represented by the set of products $\bar{J}_j$. The intuition is that the higher the market demand is for products requiring feed j, the more limited will the availability of chemical j be. Here, the coefficient $\xi_{jj'}$ defines how much the purchase limit for chemical j is affected by the demand of chemical $j' \in \bar{J}_j$. Eqs. (31e) and (31f) are nonnegativity constraints.

In this model, Q_j^0, $Q_j^{\min}$, $W_{jt}^{\max}$, μ_{ij}, and $\xi_{jj'}$ are fixed constants, $Q_j^{\max}$ and $P_i^{\max}$ are the design variables, and P_{it} and W_{jt} are the control variables. The uncertainty lies in the demand, i.e. the uncertain parameters are D_{jt} of which there exist 16 for each time period.

In the following, we apply the proposed models to problem instances of different sizes, which are created by varying the number of time periods, N_T. The computational time limit for each problem is set to one hour (wall-clock time). The flexibility test and flexibility index problems are solved for a particular design, i.e. for specific fixed values of $Q_j^{\max}$ and $P_i^{\max}$; the results are shown in Tables 6 and 7. In order to provide an indicator for the tightness of each MILP formulation, we show both v^{MIP} and v^{RMIP}, which denote the objective function values at the optimal solutions of the MILP and its LP relaxation, respectively. Note that the interpretation of v^{MIP} varies between the different problems; while it may refer to $\chi(d)$ or $\bar{\chi}(d)$ in the flexibility test problems or to $F(d)$ or $\overline{F}(d)$ in the flexibility index problems, it may also be none of those if the MILP is not solved to optimality. The solutions of the AARO LP models are also listed in the v^{MIP}-column. Furthermore, the relative optimality gap (as defined in CPLEX) is shown for each MILP. From the computational results, we make the following observations:

- In almost all instances, the DFA and the AARO models obtained the same optimal solution. The only exception is the flexibility index problem for $N_T = 10$, where Problem (FI_{DFA}) was not solved to optimality. The TFA approach only solved the flexibility test problem for $N_T = 1$ to optimality within the given time limit; in all other instances, the TFA models failed to find the optimal solution or in some cases even a feasible solution (see flexibility test for $N_T = 8$ and $N_T = 10$).

- For the larger instances, the time required by the AARO LP models to solve the flexibility test and flexibility index problems was often about one order of magnitude shorter than the time required by the DFA models.

- Compared to the DFA and AARO models, the TFA models exhibit significantly smaller numbers of constraints and continuous variables. However, recall that the TFA MILP models have m binary variables, while the DFA

MILP models have n_θ binary variables; since there are considerably more constraints than uncertain parameters in this problem, the TFA models have larger numbers of binary variables.

- The comparison between the v^{RMIP}-values of the TFA and DFA models indicates that the TFA models have significantly weaker relaxations, in part because of the big-M constraints. This is the primary reason for the better computational performance of the tighter DFA MILP models.

- It should be mentioned that although in many instances, $v^{\mathrm{RMIP}} = v^{\mathrm{MIP}}$ for the DFA models, it is often the case that the LP relaxation does not result in an integer solution. In such a case, the problem does not solve at the root node and further branching is needed.

- In all instances, when solving the flexibility index problem using formulation ($\mathrm{FI}_{\mathrm{TFA}}$), the lower bound did not improve (i.e. remained zero) during the branch-and-bound process, even when a depth-first branching strategy was applied. This observation implies that there is sufficient flexibility in the model such that even with only one binary variable being relaxed, there exists a feasible solution with $\delta = 0$. This special structure of the problem has the consequence that a very large number of nodes in the branch-and-bound tree have to be examined in order to prove optimality.

Table 6: Flexibility test results for Example 3.

N_T	Model	# of Constraints	# of Cont. Variables	# of Bin. Variables	v^{RMIP}	v^{MIP}	Gap [%]	Solution Time [s]
	(FT_{TFA})	538	369	152	0.68	−8.24	0	31
1	(FT_{DFA})	7,345	2,584	16	−8.24	−8.24	0	0.3
	(FT_{AARO})	2,584	5,682			−8.24		0.2
	(FT_{TFA})	1,074	737	304	1.98	−8.24	58	3,600
2	(FT_{DFA})	29,281	10,033	32	−7.00	−7.00	0	1
	(FT_{AARO})	10,032	22,625			−7.00		1
	(FT_{TFA})	2,146	1,473	608	3.78	−8.24	146	3,600
4	(FT_{DFA})	116,929	39,520	64	−5.23	−5.23	0	3
	(FT_{AARO})	39,520	90,305			−5.23		1
	(FT_{TFA})	3,218	2,209	912	4.68	−8.24	157	3,600
6	(FT_{DFA})	262,945	88,464	96	−4.33	−4.33	0	55
	(FT_{AARO})	88,464	203,041			−4.33		5
	(FT_{TFA})	4,290	2,945	1,216	5.18	n/a	n/a	3,600
8	(FT_{DFA})	467,329	156,864	128	−3.85	−3.85	0	155
	(FT_{AARO})	156,864	360,833			−3.85		13
	(FT_{TFA})	5,362	3,681	1,520	5.38	n/a	n/a	3,600
10	(FT_{DFA})	730,081	244,720	160	8.0	−3.64	0	468
	(FT_{AARO})	244,720	563,681			−3.64		26

We now consider a design problem in which the storage and production capacities, represented by the design variables $Q_j^{\max}$ and $P_i^{\max}$, can be expanded

Table 7: Flexibility index results for Example 3.

N_T	Model	# of Constraints	# of Cont. Variables	# of Bin. Variables	v^{RMIP}	v^{MIP}	Gap [%]	Solution Time [s]
1	(FI_{TFA})	538	369	152	0.0	8.01	100	3,600
	(FI_{DFA})	7,345	2,584	16	8.01	8.01	0	0.3
	(FI_{AARO})	2,584	3,249			8.01		0.2
2	(FI_{TFA})	1,074	737	304	0.0	8.01	100	3,600
	(FI_{DFA})	29,281	10,033	32	4.77	4.77	0	1
	(FI_{AARO})	10,032	12,898			4.77		1
4	(FI_{TFA})	2,146	1,473	608	0.0	11.70	100	3,600
	(FI_{DFA})	116,929	39,520	64	2.45	3.20	0	5
	(FI_{AARO})	39,520	51,394			3.20		10
6	(FI_{TFA})	3,218	2,209	912	0.0	15.00	100	3,600
	(FI_{DFA})	262,945	88,464	96	1.62	2.65	0	104
	(FI_{AARO})	88,464	115,489			2.65		49
8	(FI_{TFA})	4,290	2,945	1,216	0.0	12.35	100	3,600
	(FI_{DFA})	467,329	156,864	128	1.19	2.39	0	723
	(FI_{AARO})	156,864	205,185			2.39		155
10	(FI_{TFA})	5,362	3,681	1,520	0.0	15.00	100	3,600
	(FI_{DFA})	730,081	244,720	160	0.93	2.32	33	3,600
	(FI_{AARO})	244,720	320,481			2.30		408

in order to minimize the total expected cost, which is approximated by nine representative scenarios. The problem is solved for two cases, one with N_T = 4 and the other with N_T = 8; the results are shown in Table 8. Since the formulation (FT_{TFA}) seems to be unsuitable for performing the flexibility test for this problem according to the results shown above, the TFA algorithm was not applied to solve the design problem. Hence, we only compare the DFA and AARO approaches.

In both instances, one can see that Algorithm DF^*_{DFA} (with initialization of critical point set) solves the problem more quickly than Algorithm DF^0_{DFA} (with empty initial critical point set) due to the smaller number of iterations. In Algorithm DF^*_{DFA}, the design problem formulation is significantly larger because

Table 8: Design under uncertainty results for Example 3.

N_T	Model/ Algorithm	Expected Cost	# of Iterations	# of Constraints	# of Cont. Variables	Solution Time [s]
4	$\mathrm{DF}^0_{\mathrm{DFA}}$	9,891	3	6,755	2,179	66
	$\mathrm{DF}^*_{\mathrm{DFA}}$	9,891	1	45,059	14,275	11
	($\mathrm{DF}_{\mathrm{AARO}}$)	9,891		45,059	92,099	7
	($\mathrm{DF'}_{\mathrm{AARO}}$)	10,037		45,059	90,371	12
8	$\mathrm{DF}^0_{\mathrm{DFA}}$	23,451	2	12,227	3,907	482
	$\mathrm{DF}^*_{\mathrm{DFA}}$	23,451	1	167,875	53,059	260
	($\mathrm{DF}_{\mathrm{AARO}}$)	23,451		167,875	364,355	16
	($\mathrm{DF'}_{\mathrm{AARO}}$)	23,644		167,875	360,899	308*

* solved with the primal simplex method

of the larger initial set of critical points; however, since it is only an LP, the added computational effort to solve it is outweighed by the benefit of solving a smaller number of flexibility test problems, which are MILPs.

In this case, solving Problem ($\mathrm{DF}_{\mathrm{AARO}}$) results in the same solutions as obtained by the DFA algorithms, yet at a considerably lower computational expense since only one single LP has to be solved. This difference in computational performance is especially apparent in the larger instance. By solving Problem ($\mathrm{DF'}_{\mathrm{AARO}}$), higher costs are achieved, which shows the suboptimality when affine control functions are imposed on the scenario set. Notice that for the instance with $N_T = 8$, the solution time for ($\mathrm{DF'}_{\mathrm{AARO}}$) is significantly larger than for ($\mathrm{DF}_{\mathrm{AARO}}$). This stark difference is due to the fact that in this particular case, Problem ($\mathrm{DF'}_{\mathrm{AARO}}$) is poorly conditioned; hence, besides scaling, higher numeric precision had to be applied in order to solve the problem.

Conclusions

In this work, we have examined for linear systems the relationship between flexibility analysis and robust optimization, which are two approaches to solving optimization problems under uncertainty that originated from different research communities (PSE and OR, respectively). Although these two research areas have been developed independently from each other, they do share some fundamental conceptual ideas, such as the use of polyhedral sets to describe the uncertainty and the worst-case approach to guarantee feasibility for every possible realization of the uncertainty.

To systematically establish the link between flexibility analysis and robust optimization, and to compare these different approaches, the three classical problems from flexibility analysis have been considered: the flexibility test problem, the flexibility index problem, and design under uncertainty with flexibility constraints. For LPs with a given general structure, two new solution approaches have been proposed, where the first derives duality-based reformulations of the traditional active-set MILP formulations, and the second applies the concept of affinely adjustable robust optimization (AARO).

The concepts that form the theoretical basis for the three different approaches—traditional flexibility analysis (TFA), duality-based flexibility analysis (DFA), and AARO—have been compared. It has become clear that AARO can be seen as a special case of flexibility analysis, however with a duality-based approach to solving the problems. It can be shown that in general, AARO is more restrictive and therefore may be overly conservative. However, it turns out that for LP models, it is often the case that AARO does predict the same level of flexibility as TFA and DFA.

The three different approaches have been applied to three numerical examples, verifying some of the theoretical properties of the proposed formulations. The results further show that DFA and AARO may be computationally more efficient than TFA. The DFA models exhibit a better computational performance because of the tightness of the MILP formulations. In the case of AARO, the main advantage is that only LPs need to be solved; furthermore, no iterative procedure is required for solving the design under uncertainty problem.

Finally, it should be noted that flexibility analysis is not restricted to models with inequalities or to linear models since it can be applied to nonlinear models with equalities. Given the analogies that have been established in this paper with robust optimization, it would be interesting to examine whether robust optimization can also be extended to nonlinear models with equalities.

Acknowledgments

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