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Similarities and Differences Between the Concepts of Operability and Flexibility: The Steady-State Case

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This article presents a comparative review on the operability and flexibility concepts and their application to process design and control. First, the operability and flexibility methodologies are summarized. Then the application of the operability framework to steady-state and dynamic systems is illustrated through the examination of several example categories such as linear and nonlinear, square and non-square systems. The flexibility approach based on the active set strategy is used to study the same examples from the flexibility point of view. The discussed results show that the operability and flexibility approaches examine a process from different perspectives and provide valuable complementary information. *AIChE J,* 56: 702–716, 2010
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Introduction

Challenges in process operations come from the constraints imposed on the process design, the desire to change operating conditions (production rate, product qualities), and several sources of uncertainties. Specifically, these uncertainties are expected process disturbances related to variability of process parameters during operation and plant-model mismatch. These issues of input and output constraints and parametric and other uncertainties can give rise to process infeasibilities.

Determining the conditions under which the design is feasible and safe has been recognized as one of the important problems in process systems engineering. In the early 1980s, Swaney and Grossmann[1] defined the flexibility index (FI) to provide a measure of the feasible operating region in the space of the uncertain parameters, assuming that expected deviations are estimated in the positive and negative directions of each parameter from its nominal value. Simply stated, the FI corresponds to the maximum deviation of the uncertain parameters from their nominal values, by which feasible operation can be guaranteed with the proper manipulation of the control variables. Since then, a series of publications has mainly focused on improving and extending the use of this index in process design. Some concerns appear in the design of new materials where the constraints have the form of property functions. The presence of hard constraints in any operability analysis is the reassurance of safe operation. However, these constraints can be very limiting in terms of the available operating ranges. Thus, it is of major

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benefit to be able to identify as precisely as possible the feasible operating ranges to avoid limiting the operation to narrow conditions and losing the capability of performing any profit optimization studies.

Even though the effect of the process design on the control qualities of a plant has been recognized for several decades, substantial efforts to integrate process design and process control have only been initiated during the last two decades. Specifically, it is desirable to operate the process outputs at specified ranges, represented by the desired output set (DOS), and to compensate for the disturbances within an expected disturbance set (EDS). These two tasks should be accomplished using the limited control action available, given by the available input set (AIS). To quantify the operability characteristics of a prospective process design and its integration with process control, Vinson and Georgakis[2,3] proposed a simple, yet powerful, approach that focuses its attention on the constrained ranges of the input and output variables. In this approach, the ability to achieve the process control objectives for a specific design is quantified by calculating the achievable output set (AOS), which represents the output ranges that can be achieved using the inputs in the AIS. Moreover, the required input ranges to achieve the entire DOS in the presence of disturbances can also be calculated and it is represented by the desired input set (DIS). Based on these variable sets, the operability index (OI) was defined in the input and output spaces as a measure of the inherent operability of a process design. This measure is independent of the choice of the controller and provides a systematic way of ranking competing process designs. It also provides insight into the aspects of the process design that can be modified to improve its operability and identifies safe operating regions and tolerable disturbances with the available inputs. This methodology has been proven to be effective for both linear[2,3] and nonlinear processes,[4,5] consisting of a single unit or one overall plant,[6] and has also been extended to dynamic systems.[7]

Variability consistently exists in industrial process plants, and changing conditions during operation can give rise to suboptimality and even infeasibility of the deterministic solutions. Therefore, plant flexibility has been recognized to represent one of the important features in the operability of production processes. In the last two decades, the problem of determining the operating range for a feasible and safe operation has been the subject of an extensive list of publications in the literature. The areas of feasibility and flexibility basically cover: (i) a feasibility test that requires constraint satisfaction over a specified space of uncertain parameters; (ii) a FI associated with a given design that represents a quantitative measure of the range of uncertainty space that satisfies the feasibility requirement; and (iii) the integration of design and operations where trade-offs between design cost and plant flexibility are considered.

The objective of this work is to present a preliminary review on the comparative application of operability and flexibility concepts to process control and process design. Initially, a review on the operability framework for steady-state and dynamic systems is presented. The application of this methodology is illustrated through the examination of several examples characterizing different system categories, such as linear and nonlinear, square and non-square systems. The same examples are also examined from the flexibility point of view using tools based on the active set strategy.[8] The results discussed show that operability and flexibility approaches examine a process from different perspectives and provide valuable complementary information.

Process Operability: Summary of Prior Work

Steady-state analysis

Steady-state operability is a necessary condition for overall process operability, which should be subsequently complemented by dynamic operability. As briefly described earlier, Vinson and Georgakis[3] introduced the operability concepts to enable the assessment of the steady-state operability of low-dimensional linear and nonlinear square processes. The linear analyses were based on steady-state process gain matrices, whose gains provide insight into the inherent operability of a process, the degree of interaction among all the process variables, and the direction of this interaction. The nonlinear analyses were based on first principles models, typically involving mass transfer, energy transfer, and reaction kinetics. The OI was presented to provide an operability measure for multivariable systems in addition to a geometrical interpretation for systems with dimensionality lower than or equal to 3D. This measure was further proven to be independent of the inventory control structure selected.[9] This property enables its quantification during the process synthesis stage before the selection of a process control structure, permitting the comparison of operability between competing designs. The steady-state operability concepts were extended to nonlinear reactor systems [continuous stirred tank reactors (CSTR) and plug flow reactors (PFR)] and some of the computational methods for such systems were discussed.[4] The operability of CSTR systems was also investigated[5] using the steady-state[3] and dynamic operability concepts.[7] In the same work,[5] non-square cases with extra degrees of freedom (i.e., processes with more input variables than set-point controlled outputs) were considered. An overview of the operability concepts up to this point can be found in prior publications.[10,11] Also, see Refs. 12–17 for process operability approaches developed by several other research groups.

For high-dimensional systems, an extension of the operability framework to specifically address large-scale plant-wide nonlinear systems at the steady state was proposed,[6] in which the focus was limited to a few selected process outputs related to production, while maintaining all the other critical variables within constraints. Moreover, the original square operability framework was extended to high-dimensional square and non-square linear systems by Lima and Georgakis (submitted). The same authors introduced two interval operability approaches to tackle non-square systems with more outputs than inputs (Lima and Georgakis, submitted).[18] For these systems, which have fewer degrees of freedom available than the number of controlled outputs, set-point control is not possible for all the outputs and some of them must be controlled at intervals or ranges. Specifically, an iterative approach was first proposed to provide a systematic way of designing the feasible output constraints to be used in the control of non-square systems.[18] However, this methodology is limited by its computational cost, when the problem dimensionality increases, and an optimization-based approach using a linear programming (LP) framework was developed to deal with higher-dimensionality problems (Lima and Georgakis, submitted). This approach has been applied to industrial-scale chemical processes, which are high-dimensional non-square systems, controlled by model predictive controllers (MPC).[19]

Dynamic analysis

Process dynamic characteristics should be considered to enable a complete assessment of process operability. Issues of whether a disturbance can be rejected quickly enough or a set-point change can be implemented within a desired time frame must be taken into account. The extension of the steady-state operability concepts to dynamic systems was performed by Uzturk and Georgakis.[7] Specifically, a dynamic operability measure was introduced, and an optimization-based approach was developed, to fully assess the operability characteristics of processes. In this approach, an optimal control problem is solved to find the minimum time within which the process can respond to a disturbance or move to a new operating point considering the available input ranges. Thus, the solution of this problem represents an upper bound for the achievable control performance of a process enabling the identification of the inherent operability characteristics of the corresponding process. Using this framework, the steady-state and dynamic operability of CSTR systems was investigated, and non-square problems with extra degrees of freedom were considered.[5] An overview of the steady-state and dynamic operability concepts and definitions is presented in "Operability: The Basic Concept" section.

Process Flexibility: Summary of Prior Work

Several approaches exist in the literature that address the feasibility test and FI problems. The flexibility and feasibility analysis introduced by Grossmann and coworkers has been proved to be a powerful and, in most cases, the only approach available to identify the uncertainty ranges where the design, of a process or material, is feasible to operate or function. Halemane and Grossmann[20] proposed the direct search method that explicitly enumerates all the parameter set vertices. Swaney and Grossmann[1,21] proposed two algorithms: a heuristic vertex search and an implicit enumeration scheme to avoid the explicit vertex enumeration. Both algorithms rely on the assumption that critical parameter values are at the vertices. To circumvent this limitation, Grossmann and Floudas[8] proposed a solution approach based on the following ideas: (i) the inner optimization problem is replaced by the Karush-Kuhn-Tucker optimality conditions (KKT); and (ii) the discrete nature of the selection of the active constraints is used by introducing a set of binary variables to express if a specific constraint is active. Based on these ideas, the feasibility test and FI problems can be reformulated as mixed-integer optimization problems, either linear or nonlinear depending on the nature of the constraints. Saboo et al.[22] proposed an alternative approach by introducing the resilience index (RI). In an attempt to determine the probability of feasible operation, the stochastic FI was introduced by Pistikopoulos and Mazzuchi[23] and Straub and Grossmann.[24] Dimitriadis and Pistikopoulos[25] extended the steady-state flexibility analysis framework to incorporate time-varying uncertainties. The dynamic feasibility and flexibility problems were formulated as two-stage, semi-infinite, dynamic optimization problems with an infinite number of decision variables. Bansal et al.[26] extended the concept of stochastic flexibility to linear dynamic systems, where uncertain parameters are described by Gaussian probability distribution functions. Mohideen et al.[27] introduced an integrated framework for flexibility and controllability at the synthesis/design stage of dynamic systems under uncertainty. In their later work,[28] they extended that framework for operability taking into account robust stability criteria. Bansal et al.[29] presented a case study of a multicomponent distillation system to demonstrate: (i) how the process and control design, involving both discrete and continuous decisions, can be simultaneously optimized; and (ii) mixed-integer dynamic optimization problems, involving thousands of differential-algebraic equations, can be solved using state-of-the-art algorithms and technology. Pintarič and Kravanja[30] proposed a sequential two-stage approach which can handle flexibility and some aspects of operability by the synthesis of chemical processes with mixed-integer nonlinear programming (MINLP). In the work of Konukman and Akman,[31] flexibility and operability issues of a heat-exchanger network (HEN) were investigated with rigorous simulations using the process flowsheet simulator HYSYS for a HEN-integrated natural gas turbo-expander plant (TEP) operating under ethane-recovery mode.

A significant number of contributions has been made in the area of dynamic FI, and its integration with control, from Pistikopoulos' research group. A detailed overview of the technologies dedicated to the integration of process design and process control, and the optimization-based advances developed by his group, can be found in the work of Sakizlis et al.[32] Another approach for the integration of process design and control using dynamic flexibility analysis was developed by Malcolm et al.[33] Ostrovsky et al.[34] proposed a branch and bound approach based on the evaluation of upper and lower bounds of the feasibility measure. Although the suggested bounding problems are simpler than the original feasibility test problem, they correspond to bilevel optimization problems where global optimality cannot be guaranteed using local optimization methods. Considerable amount of effort has been made to address the feasibility and flexibility of nonconvex problems. Goyal and Ierapetritou[35] presented a systematic framework for an accurate approximation of the feasible region, or operating envelope, of a given design based on the basic idea of approximating it from the inside using the simplicial approximation approach and from the outside using the tangent planes at specific boundary points. Floudas et al.[36] presented a systematic and rigorous approach for the efficient solution of the feasibility test and FI problems for a given design. This approach is based on the concept of feasible domain relaxation and the basic principles of the deterministic global optimization algorithm αBB. The main feature of this presented approach is that it guarantees convergence to the global optimal solution for problems that are described by general nonconvex constraints. Banerjee and Ierapetritou[37] proposed a feasibility evaluation method that can be applied to any convex, nonconvex, or even disjoint problems. It considers the feasible region as an object and applies surface reconstruction ideas to capture and define the shape of the object. In a recent work of Moon et al.,[38] a parallel hybrid algorithm was proposed based on stochastic search in conjunction with a nearest constraint projection technique. The algorithm deploys a stochastic approach to search the design space globally, while using local gradient information to explore a reduced state variable space.

A brief overview of the mathematical formulations of the feasibility test and FI for a given design is presented in ''Flexibility Approach'' section (''Formulation'' section). ''Active Set Strategy'' section describes the basic steps of the approach proposed by Grossmann and Floudas,[8] which is mainly used in this article. All the MINLP problems in this article are solved using local optimization solvers because the purpose of this work is to illustrate the concepts of the FI and how the results are compared with the information obtained using operability analysis.

Operability: The Basic Concept

The steady-state operability analysis aims to determine whether the input ranges are sufficient to achieve the desired output ranges, in the presence of expected disturbances, using the steady-state process model. The availability of this model, which relates process inputs and disturbances to the outputs variables, is one of the basic requirements of the operability framework. For the purpose of this article, a general state-space model representation (**M**) for linear and nonlinear systems is used:

$$\mathbf{M}: \begin{cases} \frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x},\mathbf{u},\mathbf{d}) & (1) \\ \mathbf{y} = \mathbf{g}(\mathbf{x},\mathbf{u},\mathbf{d}) & (2) \\ \mathbf{h}_1(\frac{d\mathbf{x}}{dt},\mathbf{x},\mathbf{y},\dot{\mathbf{u}},\mathbf{u},\mathbf{d}) = 0 & (3) \\ \mathbf{h}_2(\frac{d\mathbf{x}}{dt},\mathbf{x},\mathbf{y},\dot{\mathbf{u}},\mathbf{u},\mathbf{d}) \le 0 & (4) \end{cases}$$

where $\mathbf{x} \in \Re^{n_s}$, $\mathbf{u} \in \Re^m$, $\mathbf{d} \in \Re^q$, and $\mathbf{y} \in \Re^n$ are the state, input, disturbance, and output vectors, respectively. The two linear or nonlinear maps **f** and **g** are of the following dimensionality:

$$\mathbf{f}: \Re^{n_s+m+q} \rightarrow \Re^{n_s}$$

$$\mathbf{g}: \Re^{n_s+m+q} \rightarrow \Re^{n}$$

The equality and inequality constraints in Eqs. 3 and 4 represent the process, product, and safety specifications. They may be applicable to the whole process history or only at the steady state. In particular, the time-dependent constraints are important in the dynamic operability analysis.

Set-point operability

The set-point operability concepts were introduced for the study of square ($n = m$) systems.[3] These concepts are based on some key operating sets that are defined here. The AIS is the set of values that the process input variables can take based on the design and constraints of the process. For an $n \times m \times q$ (outputs × inputs × disturbances) system:

$$\text{AIS} = \{\mathbf{u} | u_i^{\min} \le u_i \le u_i^{\max}; 1 \le i \le m\}$$

Examples of these variables are valves that can be manipulated during process operation. Moreover, the DOS is given by the desired operating window for the process outputs and it is represented by:

$$\text{DOS} = \{\mathbf{y} | y_i^{\min} \le y_i \le y_i^{\max}; 1 \le i \le n\}$$

These output variables could represent product qualities, reactor temperature and conversion, and the production rate of a chemical process. The DOS should also be based on market demand, safety considerations, and emission regulations. Finally, the EDS represents the values of the disturbances:

$$\text{EDS} = \{\mathbf{d} | d_i^{\min} \le d_i \le d_i^{\max}; 1 \le i \le q\}$$

Examples of these disturbances are process uncertainties, including parameters at the design stage, such as heat transfer coefficients, reaction rate constants, and physical properties; or parameters during operation, such as quality and flow rates of feed streams, catalyst activity, heat exchanger fouling, ambient temperature fluctuations, and plant-model mismatch. By solving the process model for the entire AIS, one can obtain the AOS as the union of all the output points that can be achieved. The AOS obtained for the given AIS (subscript u), fixing the disturbances at their nominal values $\mathbf{d}^N$, is represented here by $\text{AOS}_u(\mathbf{d}^N)$ and is mathematically defined as follows:

$$\text{AOS}_u(\mathbf{d}^N) = \left\{\mathbf{y} | M(\dot{\mathbf{x}} = 0, \dot{\mathbf{u}} = 0, d = d^N); \forall \mathbf{u} \in \text{AIS}\right\} \quad (5)$$

Based on these definitions, the servo OI in the output space (subscript y) is the following:

$$\text{s} - \text{OI}_y = \frac{\mu(\text{AOS}_u(\mathbf{d}^N) \cap \text{DOS}}{\mu(\text{DOS})} \quad (6)$$

Here μ represents a measure of the size of the set, e.g., area for 2D and volume for 3D examples, and hypervolume for sets with higher dimensionality.

In the presence of process disturbances, the overall AOS is defined as the intersection of all the $\text{AOS}_u(\mathbf{d})$, for all possible disturbance values within the EDS (Lima and Georgakis, submitted):

$$\text{AOS} = \bigcap_{\mathbf{d} \in \text{EDS}} \text{AOS}_u(\mathbf{d}) \quad (7)$$

The overall OI in the output space follows:

$$\text{OI}_y = \frac{\mu(\text{AOS} \cap \text{DOS})}{\mu(\text{DOS})} \quad (8)$$

This index quantifies how much of the region of the desired outputs can be achieved using the available inputs in the presence of disturbances and it is particularly useful in analyzing the operability of existing process designs. If this index is less than 1, some regions of the DOS are not achievable.

To perform a similar analysis in the input space, we first define the DIS as the set of input values required to reach the entire DOS. This set is obtained by applying the inverse of the process model to the output vectors in the DOS. Thus, the DIS calculated for a given DOS (subscript y), fixing the disturbances at their nominal values $\mathbf{d}^N$, can be represented as follows:

$$\mathrm{DIS}_y(\mathbf{d}^N) = \left\{\mathbf{u}|\mathbf{M}^{-1}(\dot{\mathbf{x}} = 0, \dot{\mathbf{u}} = 0, \mathbf{d} = \mathbf{d}^N); \forall \mathbf{y} \in \mathrm{DOS}\right\} \quad (9)$$

Now, the servo OI in the input space (subscript u) is given as follows:

$$\mathrm{s-OI}_u = \frac{\mu(\mathrm{AIS} \cap \mathrm{DIS}_y(\mathbf{d}^N))}{\mu(\mathrm{DIS}_y(\mathbf{d}^N))} \quad (10)$$

This index quantifies how much of the servo DIS is covered by the AIS and can be used to propose changes to a new or an existing plant design to enlarge the AIS, in case its value is less than 1. For linear systems, the servo OI calculated in both ways using Eqs. 6 and 10 provide the same result. However, some differences in the computed values might be observed for nonlinear systems. To investigate separately the regulatory operability of a process, a regulatory operability measure in the input space was also introduced.[3,10] The set of inputs required to compensate for the effect of the disturbances, regulating the outputs at their nominal set-point values ($\mathbf{y}^N$), is represented here by $\mathrm{DIS}_d(\mathbf{y}^N)$ and is mathematically defined as follows:

$$\mathrm{DIS}_d(\mathbf{y}^N) = \left\{\mathbf{u}|\mathbf{M}^{-1}(\dot{\mathbf{x}} = 0, \dot{\mathbf{u}} = 0, \mathbf{y} = \mathbf{y}^N); \forall \mathbf{d} \in \mathrm{EDS}\right\} \quad (11)$$

Thus, the regulatory OI in the input space is given as follows:

$$\mathrm{r-OI}_u = \frac{\mu(\mathrm{AIS} \cap \mathrm{DIS}_d(\mathbf{y}^N))}{\mu(\mathrm{DIS}_d(\mathbf{y}^N))} \quad (12)$$

Consider now the overall objective of achieving the desired output values in the DOS and also compensate for all the expected disturbances in the EDS. In the input space, the overall DIS has to be large enough to fulfill both requirements and is represented by:

$$\mathrm{DIS} = \bigcup_{\mathbf{y}\in\mathrm{DOS}} \mathrm{DIS}_d(\mathbf{y}) = \bigcup_{\mathbf{d}\in\mathrm{EDS}} \mathrm{DIS}_y(\mathbf{d}) \quad (13)$$

The overall OI in the input space can be now calculated as a function of the overall DIS and AIS:

$$OI_u = \frac{\mu(\mathrm{AIS} \cap \mathrm{DIS})}{\mu(\mathrm{DIS})} \quad (14)$$

Notice that all these indexes have values between 0 and 1. Because they express ratios of similar quantities, they are also independent of the scaling of the variables. A process is considered completely operable, with respect to each scenario, if its index is equal to 1. Thus, in set-point operability, it is desirable to reach every point in the DOS. In addition to this measure, the steady-state operability framework provides the exact subset of the desired output specifications that cannot be achieved with the current AIS. To calculate each of these indexes, and the AOS (Eq. 7), mathematical operations involving intersections of polytopes have to be performed to evaluate intersections like $\mathrm{AOS} \cap \mathrm{DOS}$. The availability of the multiparametric toolbox (MPT) in MATLAB (Mathworks™)[39] enables evaluations of such intersections for high-dimensional systems in $\Re^n$.

Interval operability

To quantify the steady-state operability of non-square linear systems, we classify the process outputs into two categories: set-point controlled: variables that are controlled at exact set-point values (production rates and product qualities); and set-interval controlled: variables that are controlled within specified ranges (pressure, temperature, and level). In the latter case, we refer to the operability as interval operability. The set-point and range variables are selected according to the process control objectives. We next define the concepts of interval operability for systems with more[5] or, most likely, fewer degrees of freedom, expressed by the number of independent input variables, than the controlled variables.[18]

Operability of Non-Square Systems

Systems with extra degrees of freedom

When a system has more input variables than set-point controlled outputs, the extra degrees of freedom available can be used to control a few other outputs at intervals or ranges. In this case, the calculation of DIS should be modified to take into account the presence of these extra degrees of freedom. The calculation strategy summarized here can be used to solve the steady-state design problem of finding the desired inputs $\mathbf{u}^*$, for given $\mathbf{y}_{\mathrm{sp}}$ and $\mathbf{d}$, as a constrained optimization problem.[5] The following objective function, $J(\mathbf{u})$, should be minimized with respect to the input variables, subject to process and performance constraints:

$$\mathbf{P1:} \begin{bmatrix} J(\mathbf{u}^*) = \min_{\mathbf{u}} J(\mathbf{u}) \\ \text{s.t} \quad \mathbf{M}\left({}^{d\mathbf{x}}/_{dt} = 0, {}^{d\mathbf{u}}/_{dt} = 0; \mathbf{y}_{\mathrm{sp}}, \text{and } \mathbf{d} \text{ given}\right) \end{bmatrix} \quad (15)$$

where the objective function is related to the cost of use of each of the inputs, and the constraints in $\mathbf{M}$ include the set of interval controlled outputs. One example of such an objective function would be a weighted sum of the squares of the inputs, where the weights would be defined according to the input costs. To calculate the overall DIS, problem **P1** should be repeated for all the set-points in the DOS and the disturbances in the EDS, where the DOS is specified only in terms of the set-point-controlled variables. The overall DIS is thus given by the union of all the solutions from these optimization problems for all pairs ($\mathbf{y}_{\mathrm{sp}}$, $\mathbf{d}$) as shown in Eq. 13 (see Ref. 5 for examples of DIS calculations). A shortcut method has also been presented to calculate the bounding box of DIS for high-dimensional plant-wide problems, where the computational cost is substantial.[6] This method focuses on a few critical output variables related to production rates and product qualities. Specifically, the achievable production output set (APOS) was defined as subset of the entire AOS. Simply stated, this set corresponds to the feasible operating region in the production-related variables that is achievable with the AIS, while maintaining all the other process variables within constraints. The dimensionality of the APOS is mainly dependent on the number of products that a plant makes and the number of independent quality variables associated with these products. Also, the desired production output set (DPOS) was defined as the DOS in the production-related output variables. Thus, an OI in the production output space (subscript p) can be now defined as follows:

$$\mathrm{OI}_p = \frac{\mu(\mathrm{APOS} \cap \mathrm{DPOS})}{\mu(\mathrm{DPOS})} \tag{16}$$

In this case, we are interested in the entire feasibility region in the production output space in addition to the index calculation. For a generic non-square system with excess of degrees of freedom, the calculation of a point on the boundary of a two-dimensional APOS was formulated as the following optimization problem:

$$\mathrm{P2}: \left[\begin{array}{l} \textbf{Maximize Production of a valuable product} \\ \text{s.t} \quad \mathbf{M}\left({}^{d\mathbf{x}}/_{dt} = 0, {}^{d\mathbf{u}}/_{dt} = 0; \text{product mix} \right. \\ \qquad \left. \text{and qualities specified; } \mathbf{d} \text{ given}\right) \end{array}\right] \tag{17}$$

By solving **P2** for different values of the quality variable in the range of interest, the upper bound of the APOS can be calculated. The lower bound can be found by repeating these calculations considering **P2** as a minimization problem. In each boundary of the APOS, the active constraints will help to find the limitations of a given plant design. This problem was originally formulated for the calculation of a two-dimensional APOS, but can also be used to obtain two-dimensional projections/slices of higher-dimensional sets. Another assumption is that the APOS is 1D convex in the fixed-variable direction, which is product quality. Varying the disturbances within the EDS, a conservative estimate of the overall APOS can be obtained by calculating the intersection of the all the APOS(**d**) obtained for all the values of disturbances entering the process:

$$\overline{\mathrm{APOS}} = \bigcap_{\mathbf{d} \in \mathrm{EDS}} \mathrm{APOS}(\mathbf{d}) \tag{18}$$

An example of the APOS calculation for the Tennessee Eastman (TE) challenging process,[40] which is plant-wide and nonlinear, can be found in Ref. 6. Note that for cases where all the outputs are production-related variables, and their number is equal to the number of inputs, AOS, DOS, and OI introduced previously would reduce to APOS, DPOS, and OI_p, respectively.

Systems with fewer degrees of freedom than controlled outputs

Non-square systems with more outputs than inputs are common in industrial chemical processes. In such systems, it is impossible to control all the outputs at specific set-points because there are fewer degrees of freedom available than the controlled variables. Thus, interval control is needed for at least some of the output variables. These intervals must be carefully defined; if they are chosen to be too narrow, the problem might be infeasible. On the other hand, if they are too wide, the desired tightness of control achieved for some of the outputs might be unsatisfactory. Thus, based on the input constraints, generally specified a priori due to the physical limitations of the process (AIS), an important task is to define the output ranges within which one can operate the process feasibly in the presence of disturbances (EDS). Because the improper selection of these constraints can make the controller infeasible, hard constraints are enforced when they are feasible and softened whenever it is necessary to retain feasibility.[41–43] However, if the output constraints are relaxed more than necessary, less tight control for some of the variables will be achieved. Looser control causes the operating point of the process to stray further away from the true economic optimum, which is often at the boundary of the acceptable region of operation. The interval operability methodology formulated in the LP framework (Lima and Georgakis, submitted) provides a method for selecting such output constraints systematically, so that they are as tight as possible and do not render the controller infeasible. This framework, which was originally developed to address high-dimensional non-square systems, can be used to tackle any input–output linear system. This method was also shown to be applicable to the online design of output constraints for non-square MPC controllers.[19] This enables the online adaptation of the control objectives to make it feasible for the magnitude of the disturbances that enter the process during operation.

As mentioned earlier, the AIS, DOS, and EDS are subsets of $\Re^m$, $\Re^n$, and $\Re^q$, respectively. Thus, for non-square systems with more outputs than inputs, the $\mathrm{AOS}_u(\mathbf{d}^N)$ is a subset of an m-dimensional manifold in $\Re^n$. Varying the process disturbance, which can take values within the EDS (a subset of a q-dimensional manifold), the $\mathrm{AOS}_u(\mathbf{d}^N)$ is shifted in the $\Re^n$ space along directions determined by the linear disturbance-to-output model and by the values of the disturbance vector. Here, the extreme cases characterized by values of the disturbance vector at the vertices of the EDS are of primary interest. For the non-square case, the AOS for interval operability (subscript I) is defined as the union of all shifted locations for all possible disturbance values:

$$\mathrm{AOS}_\mathrm{I} = \bigcup_{\mathbf{d} \in \mathrm{EDS}} \mathrm{AOS}_u(\mathbf{d}) \tag{19}$$

which is a subset of $\Re^n$. To calculate the tightest operable output ranges, the achievable output interval set (AOIS) was defined as the smallest possible feasible set of output constraints that can be achieved at the steady state with the available ranges of the manipulated variables, when the disturbances attain any values within their expected ranges. This set represents the minimum requirement for the output constraints for an operable system. In other words, as long as the AOIS is a subset of the DOS, the system is interval operable (AOIS) $\subseteq$ DOS).[18]

Finally, this LP-based approach was applied to perform high-dimensional AOIS calculations in $\Re^q$ for several industrial non-square processes provided by Air Products and Chemicals and DuPont.[19] The algorithm of this calculation, which takes into account different target operating points and relative output weights, is given in detail by (Lima and Georgakis, submitted). The effectiveness of this approach is demonstrated here through the Dryer Control Problem (provided by DuPont) in "High-Dimensional and Non-Square Linear System: Dryer Control Problem" section.

Dynamic Operability

Based on the steady-state concepts described earlier, a dynamic operability framework was formulated.[7] For the purpose of this framework, a quantitative dynamic performance measure of operability was defined as the shortest time required for a system to settle to the desired set-point, after a set-point change and/or a disturbance occurrence. This measure is based on the idea that the time spent away from the desired set-point is linked to potential losses due to off-specification products and economic penalties for nonoptimal performance. An approach based on the minimum-time optimal controller was developed for assessing the inherent limitations of the process, independently of the feedback controller used. This approach is based on the assumption that a feedback controller exists that will deliver a closed-loop dynamic operability close to the one calculated by the use of the optimal open-loop controller. Because of space limitations, we will not attempt to compare the similarities and differences between dynamic operability and flexibility in this article.

Flexibility Approach

Formulation

Halemane and Grossmann[20] proposed a feasibility measure for a given design based on the worst points for feasible operation, which can be mathematically formulated as a max-min-max optimization problem as follows:

$$\chi(r) = \underset{\theta\in\Theta}{\text{Max}}\ \min_{u}\ \max_{j\in J, i\in I}\left\{g_j(r,u,x,\theta)\leq 0\right\}$$
$$\text{s.t}\ h_i(r,u,x,\theta) = 0$$

where the function $\chi(r)$ represents a feasibility measure, r corresponds to the vector of design variables, u is the vector of control variables, x is the vector of state variables, and θ is the vector of uncertain parameters. If $\chi(r) \leq 0$, design r is feasible for all $\theta \in \Theta$, whereas if $\chi(r) > 0$, the design cannot operate for at least some values of $\theta \in \Theta$.

The above max-min-max problem defines a nondifferentiable global optimization problem which can be reformulated as the following two-level optimization problem.

$$\chi(r) = \underset{\theta\in\Theta}{\text{Max}}\ \Psi(r,\theta) \text{where } \Psi(r,\theta) = \min_{u,\mu}\mu$$
$$\text{s.t}\ h_i(r,u,x,\theta) = 0, i\in \text{I} \ \text{ and } \ g_j(r,u,x,\theta) \leq \mu, j \in \text{J}$$

where the function $\Psi(r,\theta) = 0$ defines the boundary of the feasible region in the space of the uncertain parameters θ.

The design of FI problem as introduced by Swaney and Grossmann[1] can be reformulated to represent the determination of the largest hyper-rectangle that can be inscribed within the feasible region of the design. Following this idea, the mathematical formulation of the flexibility problem has the following form:

$$\begin{aligned}&\text{FI} = \min\ \delta \quad s.t. \quad \Psi(r,\theta) = 0 \text{ and } \Psi(r,\theta) = \min_{u}\mu \\ &\text{with} \quad h_i(r,u,x,\theta) = 0, i\in \text{I}; \quad g_j(r,u,x,\theta) \leq \mu,\ j\in \text{J} \\ &\text{and} \quad \Theta(\delta) = \{\theta|\theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N - \delta\Delta\theta^+\}; \delta \geq 0\end{aligned} \tag{20}$$

For the case where the constraints are one-dimensional jointly quasi-convex in θ and quasi-convex in u, it was proven by Swaney and Grossmann[1] that the point θ_c that defines the solution to (20) lies at one of the vertices of the parameter set Θ. Based on this assumption, the critical uncertain parameter points correspond to the vertices and the feasibility test problem is reformulated in the following manner:

$$\chi(r) = \underset{k\in K}{\text{Max}}\ \Psi(r,\theta^k)$$

where $\Psi(r, \theta^k)$ is the evaluation of the function $\Psi(r, \theta)$ at the parameter vertex θ^k and $\mathbf{K}$ is the index set for the 2^{n_θ} vertices for the n_θ uncertain parameters θ. In a similar fashion for the FI, the problem in Eq. 20 is reformulated in the following way:

$$\text{FI} = \min_{\text{k}\in\text{K}}\delta^k$$

where δ^k is the maximum deviation along each vertex direction $\Delta\theta^k$ ($k \in \mathbf{K}$) and is determined by the following problem:

$$\begin{aligned}\delta^k = &\max_{\delta,u}\delta \\ &\text{s.t.}\ h_i(r,u,x,\theta) = 0, i\in \text{I and } g_j(r,u,x,\theta) \leq \mu, \quad j\in \mathbf{J} \\ &\theta = \theta^N + \Delta\theta^k, \quad \delta \geq 0\end{aligned}$$

Active set strategy

Grossmann and Floudas[8] proposed the active set strategy for the solution of the above reformulated problems based on the property that for any combination of $m+1$ binary variables that is selected (i.e., for a given set of active constraints), all the other variables can be determined as a function of θ. They proposed a procedure of systematically identifying the potential candidates for the active sets based on the signs of the gradients $\nabla_u g_j(r,u,x,\theta)$. The inner feasibility function subproblem is relaxed by providing valid underestimating functions of the original constraints. The resulting formulation is then solved by applying the KKT optimality conditions that transform the FI problem into a single-stage MINLP optimization problem as follows:

$$\begin{aligned}&\text{FI} = \min\delta \\ &\text{s.t.}\ h_i(r,u,x,\theta) = 0,\ i\in \text{I and } g_j(r,u,x,\theta)+s_j = 0,\ j\in\text{J} \\ &\sum_{j=1}^{J}\lambda_j\frac{\partial g_j}{\partial u}+\sum_{i=1}^{I}\beta_i\frac{\partial h_i}{\partial u} = 0 \text{ and } \sum_{j=1}^{J}\lambda_j\frac{\partial g_j}{\partial x}+\sum_{i=1}^{I}\beta_i\frac{\partial h_i}{\partial x} = 0 \\ &\sum_{j=1}^{J}\lambda_j = 1,\ \lambda_j - z_j \leq 0,\ s_j - U(1-z_j)\leq 0, \text{ and } \sum_{j=1}^{J}z_j = m+1 \\ &\theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N - \delta\Delta\theta^+, \text{ and } \delta\geq 0, z_j = \{0,1\}, \lambda_j, s_j \geq 0\end{aligned} \tag{21}$$

where s_j are the slack variables of design inequalities; λ_j and β_i are the associated Lagrange multipliers; and z_j are 0,1 variables (z_j =1 if constraint j is active; 0 otherwise). The resulting problem can be solved using a local MINLP optimizer (e.g., DICOPT, MINOPT). Note that for the case when nonconvexity exists, this formulation does not provide an accurate value of the FI. However, the aim of this work is to illustrate the similarities and differences between the concepts of operability and flexibility analysis, instead of focusing on the solution methodology. Hence, a simplified solution can serve this purpose.

Case Studies

In this section, three examples are addressed using the operability and flexibility approaches. The results obtained are compared to illustrate how different information can be provided by these two methodologies. The first two examples are both non-square linear systems. The example in "Simple Non-square Linear System" section is a simple system with 2 outputs, whereas the example in "High-Dimensional and Non-Square Linear System: Dryer Control Problem" section is a high-dimensional Dryer Control Problem provided by DuPont. The last example, which is a shower problem, represents a steady-state nonlinear system.

Simple non-square linear system

Consider a simple non-square linear system with 2 outputs, 1 input, and 1 disturbance variable, described by the following model and sets[18]:

$$\begin{pmatrix} \delta y_1 \\ \delta y_2 \end{pmatrix} = \begin{pmatrix} 1.41 \\ 0.66 \end{pmatrix} \delta u_1 + \begin{pmatrix} -0.6 \\ 0.4 \end{pmatrix} \delta d_1 \tag{22a}$$

with

$$\begin{aligned} &\delta \mathbf{y} = \mathbf{y} - \mathbf{y}_{ss}; \delta u_1 = u_1 - u_{1,ss}; \delta d_1 = d_1 - d_{1,ss} \\ &\text{AIS} = \{u_1 | -1 \le \delta u_1 \le 1\} \text{ and DOS} = \{\mathbf{y} \in \Re^2 | \|\delta \mathbf{y}\|_\infty \le 1\} \end{aligned} \tag{22b}$$

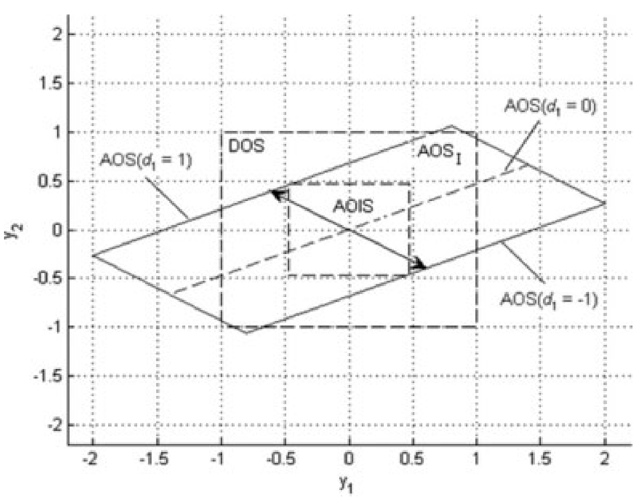

Figure 1. AOS$_I$, DOS, and AOIS for 2D example.

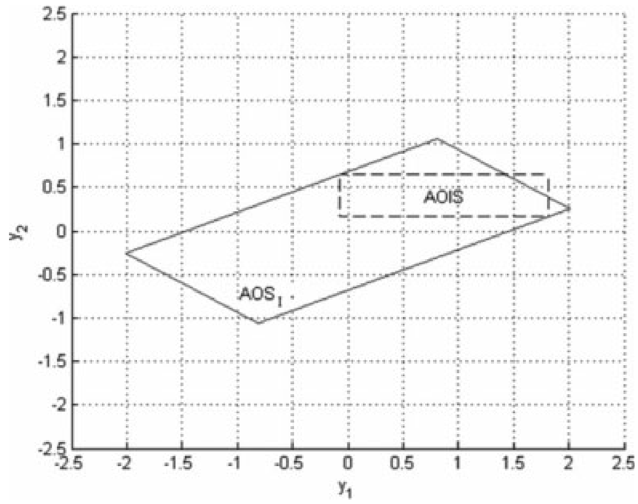

Figure 2. AOIS calculated for $\mathbf{y_0}$ = (0.5, 0.5)^T and w = (1,4)^T.

where $\delta \mathbf{y}$, δu_1, and δd_1 are deviation variables from the steady-state values for the outputs ($\mathbf{y}_{ss}$), the input ($u_{1,ss}$), and the disturbance ($d_{1,ss}$), respectively. In this example, it is assumed that the origin is the nominal steady-state point for all the variables ($\mathbf{y}_{ss} = (0,0)^T$, $u_{1,ss} = 0$, and $d_{1,ss} = 0$). Thus, for simplicity of notation, the symbol δ will be dropped here. Also, the two outputs are intended to be controlled equally tightly around their target point ($\mathbf{y}_0$), which is also at the origin.

Operability Analysis. The AOIS calculated for these specified conditions is presented in Figure 1. In the same figure, the three cases of the AOS(d_1) for $d_1 = -1$, 0, +1 are drawn parallel to each other, along with the AOS$_\text{I}$ and the DOS.

Notice that the DOS is large enough to cover the entire AOIS, which characterizes an operable system for all the disturbance values within the EDS. In fact, the DOS could be significantly reduced to achieve tighter control of the outputs as long as the AOIS remains a subset of the updated DOS. For operable systems, the amount of reduction of the original constrained region, without causing infeasibilities, is quantified by the following hypervolume ratio (HVR):

$$\text{HVR} = \frac{\mu(\text{DOS})}{\mu(\text{AOIS})}$$

where μ is a measure of the size of the corresponding polygon. For this particular example, HVR = $(2/0.94)^2$ = 4.53, which implies that the area of the constrained region could be reduced by a factor 4.53 times. Consider now that y_2 must be controlled four times tighter than y_1 around $\mathbf{y}_0 = (0.5, 0.5)^T$. In this case, the relative output weights are given by $\mathbf{w} = (w_1, w_2) = (1,4)^T$. The AOIS calculated in this case is shown in Figure 2, along with the AOS$_\text{I}$.

Flexibility Analysis. Following the procedure presented in "Active Set Strategy" section, the feasibility problem (Eq. 21) can be formulated (see Eq. A1 for the detailed equations). The resulting formulation is a MILP problem which can be solved to optimality using GAMS/CPLEX

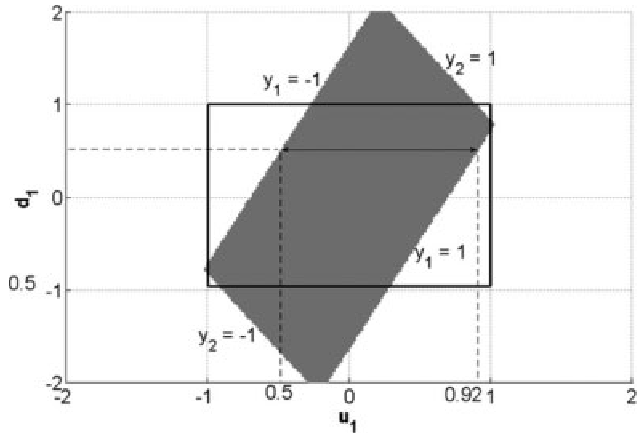

Figure 3. AIS, EDS, and DOS for 2D example.

within 0.046 CPU seconds. It is found that the objective value is 2.16, which implies that, under any disturbance d_1 between -1 and 1, there always exists an input u_1 in AIS such that the output point falls in the region of DOS. This is graphically illustrated in Figure 3. The parallelogram represents the space of input and disturbance that corresponds to the DOS, which is bounded by $-1 \leq y_1 \leq 1$ and $-1 \leq y_2 \leq 1$, whereas the AIS and EDS are represented by the square. It is trivial that when d_1 varies from -1 to 1, u_1 can be manipulated within the interval $[-1, 1]$ to obtain an output point in the DOS. For example, for the case of disturbance $d_1 = 0.5$, u_1 can take any value between -0.5 and 0.92 to achieve a desired output. An FI greater than 1 suggests that even if the disturbance exceeds EDS, a feasible operation can still be possibly achieved. In this example, the FI 2.16 indicates that the disturbance is allowed to vary from -2.16 to 2.16. On the other hand, as pointed out in operability analysis, the DOS is large enough to cover the entire AOIS. In other words, for any realization of the disturbances that belong to EDS, there always exists at least one operating point in the area of DOS. Since the system is fully operable for all the disturbance values, the FI should be larger than or equal to 1, which agrees with the result obtained from flexibility analysis.

To better illustrate the concept of flexibility, one of the coefficients in the model (Eq. 22a) has been changed to -3.6 from -0.6 as follows:

$$\begin{pmatrix} \delta y_1 \\ \delta y_2 \end{pmatrix} = \begin{pmatrix} 1.41 \\ 0.66 \end{pmatrix} \delta u_1 + \begin{pmatrix} -3.6 \\ 0.4 \end{pmatrix} \delta d_1$$

Solving this modified formulation, the FI becomes 0.67, which implies that the maximum disturbance the system can handle is $(-0.67, 0.67)$. As illustrated in Figure 4, when the disturbance $d_1 = 1$, an output that lies in the DOS cannot be achieved by manipulating the input variable u_1 in the AIS.

High-dimensional and non-square linear system: dryer control problem

The Dryer Control Problem is characterized by a high-dimensional and non-square system with 6 outputs, 4 inputs, and 2 disturbance variables. The steady-state linear model, the constraining sets, and the relative output weights that describe this process are the following:

$$\begin{pmatrix} \delta y_1 \\ \delta y_2 \\ \delta y_3 \\ \delta y_4 \\ \delta y_5 \\ \delta y_6 \end{pmatrix} = \begin{pmatrix} 9.00 & -5.10 & -0.80 & 0.31 \\ 0.06 & -0.05 & 0.03 & 0 \\ 0.70 & -0.40 & 0 & 0 \\ -44.00 & -3.00 & 3.50 & 1.56 \\ 0 & 9.60 & 0 & 0 \\ 0.60 & 0 & -0.03 & -0.13 \end{pmatrix} \begin{pmatrix} \delta u_1 \\ \delta u_2 \\ \delta u_3 \\ \delta u_4 \end{pmatrix} + \begin{pmatrix} 0.62 & 0 \\ 0 & 0 \\ 0 & 0 \\ -1.10 & 1 \\ -1.50 & 0 \\ 0.04 & 0 \end{pmatrix} \begin{pmatrix} \delta d_1 \\ \delta d_2 \end{pmatrix} \quad (23a)$$

with

$$\begin{aligned} \text{DOS} &= \left\{ \begin{matrix} \mathbf{y} \in \Re^6 | 900 \leq y_1 \leq 1000; \quad -4 \leq y_2 \leq 0; \\ -40 \leq y_3 \leq -10; \\ 100 \leq y_4 \leq 170; 1300 \leq y_5 \leq 1650; 0 \leq y_6 \leq 1 \end{matrix} \right\} \\ \text{AIS} &= \{ \mathbf{u} \in \Re^4 | 30 \leq u_1 \leq 95;\ 40 \leq u_2 \leq 95; \\ &\quad 0 \leq u_3 \leq 100; 20 \leq u_4 \leq 90 \} \\ \text{EDS} &= \{ \mathbf{d} \in \Re^2 | 30 \leq d_1 \leq 70; -30 \leq d_2 \leq 30 \} \\ \mathbf{w} &= \left[\tfrac{1}{3},\ \tfrac{1}{4},\ \tfrac{1}{4},\ 1,\ \tfrac{1}{4},\ \tfrac{1}{2} \right]^T \end{aligned} \quad (23b)$$

Operability Analysis. It is assumed initially that the steady state is at the midpoint of each of the process variable ranges and the output target is at $\mathbf{y}_0 = (950, -2, -25, 135, 1475, 0.5)^T$. The AOIS, represented by the calculated ranges around $\mathbf{y}_0$, and the constraint reduction factors (CRF) for each of the outputs in this case are presented in Table 1. These factors are calculated by the ratio between the DOS and the AOIS ranges for each of the outputs.[18] Thus, the hypervolume of the original 6D space of operation could be significantly reduced (HVR $= 5.96 \times 10^6$) without causing process infeasibilities.

Now if one wants to control the two most important output variables (y_4 and y_6) at their set-points ($y_4 = 100$ and y_6

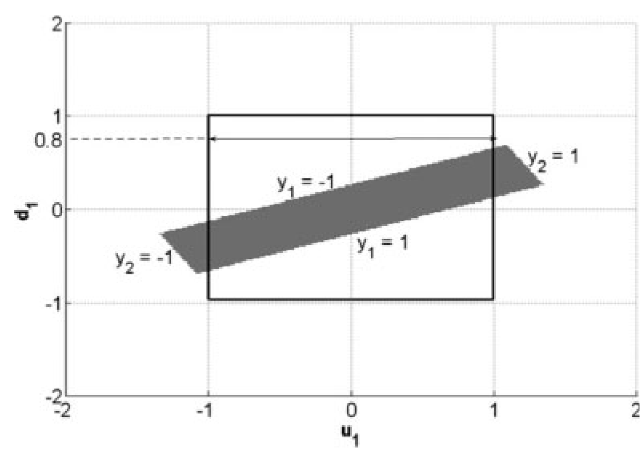

Figure 4. AIS, EDS, and DOS for modified 2D example.

Table 1. Dryer Control Problem Results: Original and Calculated Bounds (Represented by DOS and AOIS, Respectively), Target Point and Constraint Reduction Factors for Each of the Controlled Variables

Process Outputs	DOS Lower Bound	DOS Upper Bound	Target Point ($\mathbf{y}_0$)	AOIS Lower Bound	AOIS Upper Bound	CRF
y_1	900.00	1000.00	950.00	945.96	954.04	12.38
y_2	−4.00	0.00	−2.00	−2.22	−1.78	9.09
y_3	−40.00	−10.00	−25.00	−26.62	−23.38	9.26
y_4	100.00	170.00	135.00	134.05	135.95	36.84
y_5	1300.00	1650.00	1475.00	1456.20	1493.80	9.31
y_6	0.00	1.00	0.50	0.47	0.53	16.67

= 1), their weights (w_4 and w_6, respectively) must be increased. The calculated AOIS ranges and CRFs for $\mathbf{y}_0 = (960, -2, -25, 100, 1475, 1)^T$ and $\boldsymbol{w} = (1/3, 1/4, 1/4, 100, 1/4, 50)^T$ are shown in Table 2. Note that y_4 and y_6 may be practically operated at their set-points if the other variables have their constraints at least as wide as the AOIS ranges.

Flexibility Analysis. To determine the FI of the uncertain region, a MILP problem is formulated. The equations describing it are given in Eq. A2. In these equations, y_{jss} ($j = 1 \ldots 6$), u_{jss}($j = 1 \ldots 4$), and d_{jss} ($j = 1, 2$) are values of y, u, and d at steady state. The resulting MILP problem involves 20 binary variables (y) and can be solved using GAMS/CPLEX within 0.203 CPU seconds with objective value equal to 6.84, which indicates a high degree of flexibility. As shown in Figure 5, the EDS is represented by the small rectangle, while the large rectangle is the region of disturbances that can be tolerated. The EDS can be greatly enlarged without causing process infeasibilities.

This result is in a way consistent with the conclusion from the operability analysis, that the hypervolume of the 6D space of operation could be significantly reduced (HVR = 5.96×10^6) without causing process infeasibilities. The area of EDS could also be enlarged by approximately seven times and feasible operation could still be achieved.

Steady-state nonlinear example: shower problem

Consider a "shower" problem,[3] where the inputs are streams of cold ($0 \leq q_1 \leq 4$ gal/min) and hot water ($0 \leq q_2 \leq 3$ gal/min) ($u_1 = q_1$ and $u_2 = q_2$). Assume initially that the cold and hot water temperatures are fixed at $T_1 = 60$°F and $T_2 = 120$°F, respectively. These temperatures could be subjected to disturbances or uncertainties. The total flow (F) obtained from the mixture of the two streams and the outlet water temperature (T) are considered as the process outputs ($y_1 = F$ and $y_2 = T$). Moreover, the following nonlinear model relates process outputs and inputs:

$$F = q_1 + q_2 \quad \text{and} \quad T = \frac{q_1 T_1 + q_2 T_2}{q_1 + q_2} \tag{24}$$

The operating region available for the water streams characterizes the AIS. Furthermore, assume that the desired ranges of the shower total flow and temperature are $3 \leq F \leq 7$ gal/min and $74 \leq T \leq 94$°F, respectively, representing the DOS. Now consider that the hot water temperature can vary between $T_2 = 110$°F and $T_2 = 130$°F, which characterizes a disturbance of $-10 \leq d \leq 10$°F, representing the EDS. We will now analyze this problem using the operability and flexibility approaches.

Operability Analysis. Applying the process model (Eq. 24) to the AIS, the achievable values of the shower outputs in the absence of disturbances AOS($\mathbf{d} = 0$) can be calculated. This set along with the DOS is depicted in Figure 6, in which the shaded region represents the intersection of these two sets or the achievable region of the DOS. Notice that only 76% of the DOS is achievable, captured by the OI (= 0.76). Therefore, the operability framework shows that some of the desired values of the outputs (DOS) are not achievable, i.e., the initial expectations of the process design were unrealistic. It also shows what regions could be achieved and what expectations would be realistic. This is very significant for a chemical process; for instance, consider the case where the process outputs are the product quality and the production rate of a specific chemical product and the inputs are the feed flow rates of two reactants. Using the operability methodology, the amount of increase in the production rate that could be obtained in an achievable manner could be determined and an optimal production rate for a desired product quality could be calculated using the available process handles or inputs.

Now consider the hot water temperature disturbance of $-10 \leq d \leq 10$°F, which represents the EDS. The presence of such a disturbance will shift the AOS($d = 0$) according to the extreme values of the EDS (Figure 7). The intersection of all shifted locations of the AOS(d) for all values of the

Table 2. Dryer Control Problem Results for Set-Point Case: Original and Designed Bounds, Target Point and Constraint Reduction Factor for Each of the Controlled Variables

Process Outputs	DOS Lower Bound	DOS Upper Bound	Target Point ($\mathbf{y}_0$)	AOIS Lower Bound	AOIS Upper Bound	CRF
y_1	900.00	1000.00	960.00	955.09	963.21	12.32
y_2	−4.00	0.00	−2.00	−2.19	−1.73	8.70
y_3	−40.00	−10.00	−25.00	−26.67	−23.33	8.98
y_4	100.00	170.00	100.00	99.99	100.01	3598.60
y_5	1300.00	1650.00	1475.00	1452.10	1491.00	9.00
y_6	0.00	1.00	1.00	1.00	1.00	1799.30

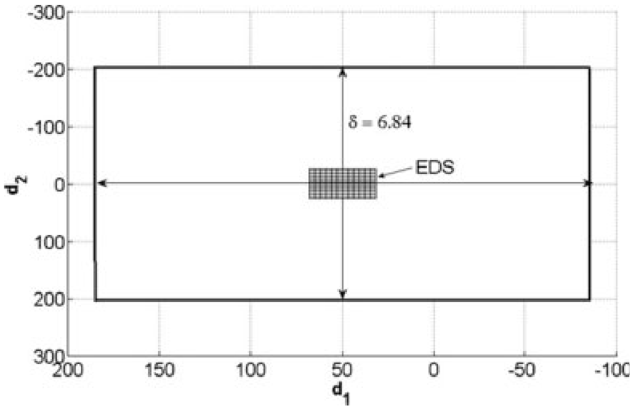

Figure 5. EDS and flexibility index for high-dimensional example.

disturbance will yield the AOS (Eq. 7), which is plotted in Figure 8, along with the DOS. Because of the presence of the disturbance in T_2, a smaller amount of the DOS is covered by the AOS (59%) than in the servo case above. This is captured by the OI (= 0.59). In a comparable example for the production of a chemical product, consider a case where one of the feed stream compositions is uncertain and dependent on an upstream process. Using this methodology, the operability quantification could still be performed and the best production rate for a product quality is determined in the presence of variations in the feed stream composition.

Flexibility Analysis. The FI can be determined with the formulation detailed in Eq. A3. In these equations, q_{1ss}, q_{2ss}, T_{2ss}, F_{ss}, and T_{ss} are steady-state values of q_1, q_2, T_2, F, and T. The above formulation is nonlinear and nonconvex because of the bilinear term q_2T_2 in the original constraints and bilinear term λ_jT_2 in the gradient KKT constraints. As presented in the work of Floudas et al.,[36] their proposed framework is able to handle problems with general nonconvex equality and inequality constraints. In this example, the nonconvex MINLP is solved using GAMS/SBB, which is based on a combination of the standard B&B method and some of the standard NLP solvers, resulting in an FI value of 3.33 within 33 nodes in 0.68 CPU seconds. Therefore, the maximum disturbance in the hot water temperature T_2 that can be handled by the system is

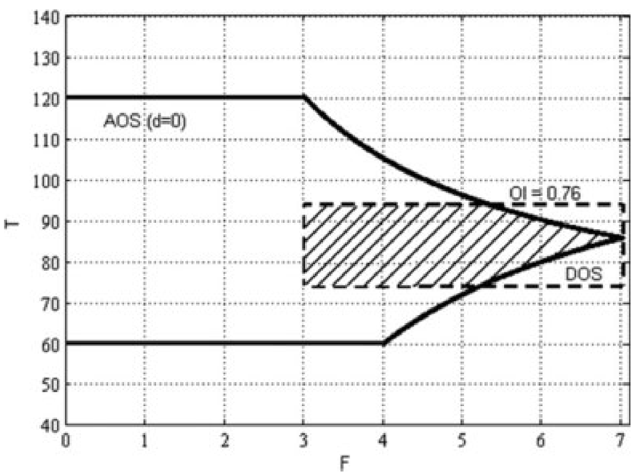

Figure 6. DOS and AOS (d = 0) for shower problem.

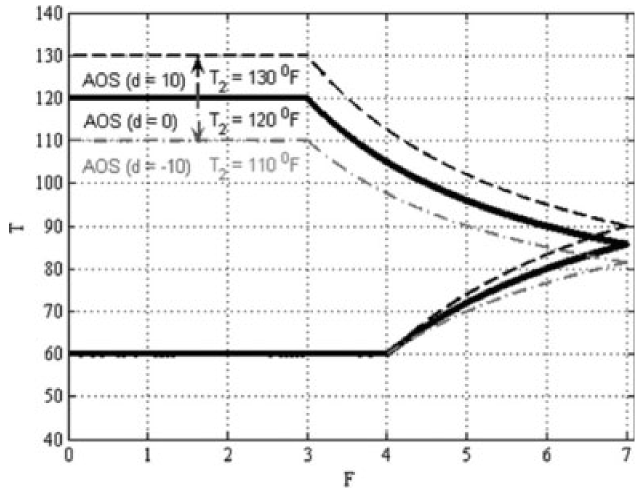

Figure 7. Shower problem: AOS shifting in the presence of a disturbance in T_2.

$-33.3 \le d \le 33.3$°F. The region in Figure 9 represents the mapping of DOS in the space of disturbance (T_2) and inputs (q_1, q_2). As shown in the figure, when T_2 takes any value between 110 and 130°F, a desired total flow and water temperature can always be achieved by adjusting the hot and cold water flows (q_1, q_2) within their available ranges. For instance, when $T_2 = 130$°F, the larger area (gray region) in Figure 10 shows the operating range of q_1 and q_2 so as to have an output in DOS, which is the intersection of plane $T_2 = 130$°F with the surface in Figure 9. Then due to the AIS $0 \le q_1 \le 4$ gal/min and $0 \le q_2 \le 3$ gal/min, the smaller area is the actual feasible operating region in which q_1 and q_2 can be adjusted to achieve a (T, F) ∈ DOS. The operability analysis of this example shows that only 59% of DOS is covered by the AOS (OI = 0.59) due to the disturbance on T_2. This result illustrates that flexibility concerns if a feasible operation can be achieved for any realization of disturbances in EDS by manipulating the inputs in AIS, whereas the focus of operability is if the entire DOS can be achieved by adjusting the inputs in AIS and disturbance in EDS. Therefore, even if the OI is less than 1, it is still possible to have an FI greater than 1.

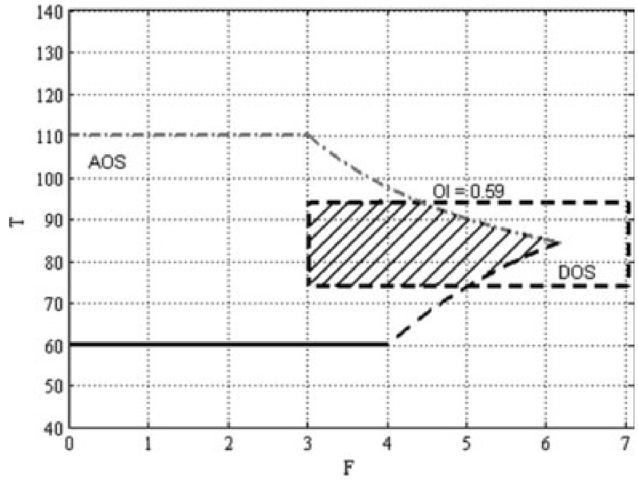

Figure 8. Operability index for shower problem with a disturbance in T_2.

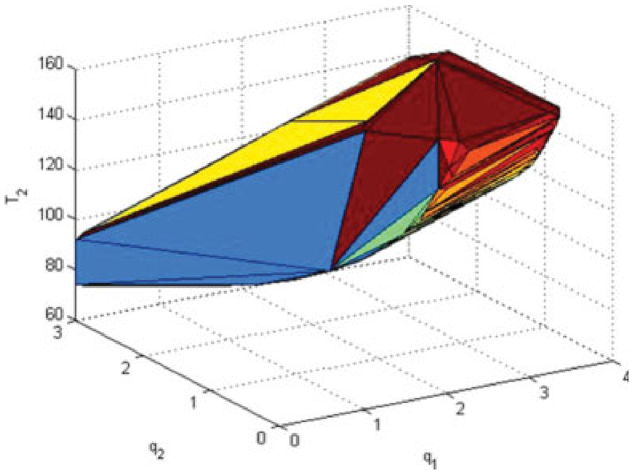

Figure 9. Projection of DOS in input and disturbance space for shower problem.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

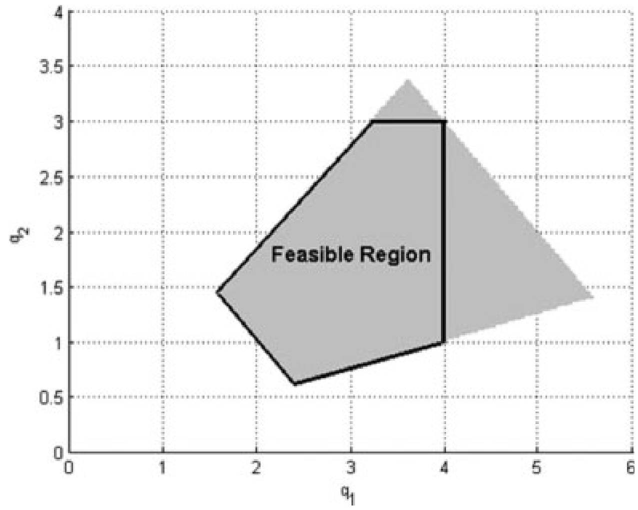

Figure 10. Feasible region of hot and cold flow for T_2 = 130°F.

Discussion of Similarities and Differences

From the examples discussed earlier, the two methodologies aim to examine similar, but not identical, process characteristics from two initially different points of view. The process operability approach is motivated by the concern of whether a process controller might not be able to achieve its mission due to limitations of the process design. On the other hand, process flexibility is concerned with whether a given process design is feasible due to the uncertainties in some of the parameters that have been used in the nominal design.

As such, operability focuses on the examination of the existing constraints in the input (manipulated or process disturbances) variables and the desirable constraints in the output variables that need to be controlled. It can also address non-square systems considering both set-point and interval control objectives. The operability of a process has been analyzed in the input space to consider whether design changes need to be made to enlarge the range of the input variables and enhance the operability of the process. Examination of the operability in the output space enables the calculation of the ranges over which the desired set-points can be varied. In the case of interval control, the recently established approach calculates the tightest possible intervals within which the outputs can be controlled for the expected ranges of disturbances.

On the other hand, the flexibility approach focuses exclusively on the calculation of the maximum size of the disturbance set that can be handled without the process being moved away from its nominal operating point. Both methods have used an extensive array of optimization tools to answer the corresponding problems that they have set forth to address. The results discussed show that the operability and flexibility approaches examine a process from different perspectives and provide valuable complementary information. Figure 11 schematically represents the interrelationships between these two concepts.

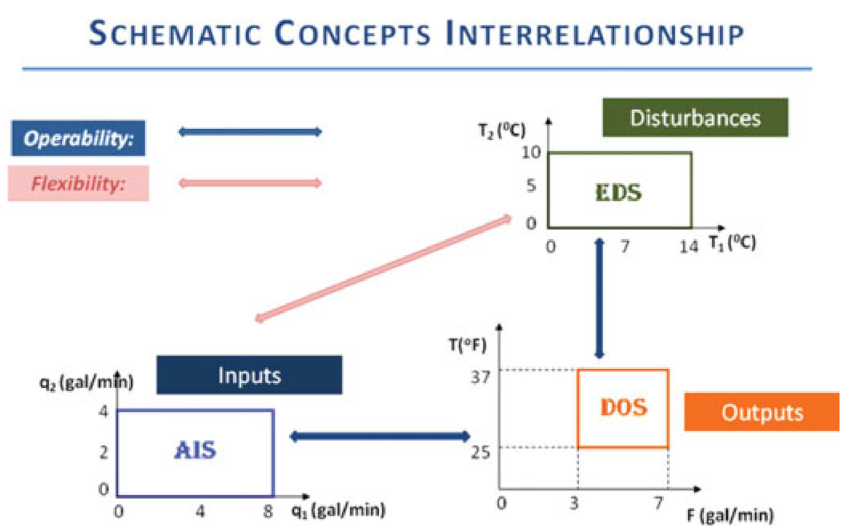

Figure 11. Schematic interrelationship: input, output, and disturbance sets as examined by the operability and flexibility concepts.

[Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Conclusions

Two similar but not identical concepts—operability and flexibility—are presented in this article. Three examples are provided to illustrate how these approaches address the same processes from different perspectives.

Set-point operability requires all the points in DOS to be reached by adjusting the input variables in the presence of disturbances. When there are fewer degrees of freedom than the controlled variables, the concept of interval operability is introduced, where some of the output variables are required to be controlled within ranges instead of set-point values. The system is considered as fully interval operable if the operable output ranges fall in the region of DOS for all the values of disturbances. In contrast to set-point operability that aims to achieve every operating point in DOS, flexibility analysis concerns itself on whether a feasible operation can be reached in the presence of disturbances in EDS. Thus the concept of flexibility is related to interval operability, but the former focuses on finding if the operation at a point is feasible in the presence of disturbances. The latter examines whether all the points in the desirable output ranges are operable in the presence of disturbances and with the available ranges of inputs.

Notation

d = disturbance variables
FI = flexibility index
$\mathbf{f}$, $\mathbf{g}$, $\mathbf{h}$ = general linear or nonlinear functions
I, J = index set of i, j
i, j = index of constraints
$\mathbf{K}$ = index set of k
k = index of vertices
$\mathbf{M}$ = general state-space model
m = number of input variables
n = number of output variables
n_s = number of state variables
OI = operability index
P1, **P2** = operability optimization problems
q = number of disturbance variables
r = design variables
s = slack variables
t = time variable
u = input or control variables
w = relative output weights
x = state variables
y = output variables
z = binary variables
λ, β = Lagrange multipliers
Θ = parameter set of θ
θ = uncertain parameters

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Appendix

In this appendix, we provide the detailed equations that define the optimization problem that represents the flexibility calculations.

The equations defining the flexibility problem of the example in "Simple Non-square Linear System" section are as follows:

$$
\begin{aligned}
&\mathrm{FI} = \min\ \delta \\
&\text{s.t. } 1.41u_1 - 0.6d_1 - 1 + s_1 = 0, -1.41u_1 + 0.6d_1 - 1 \\
&+s_2 = 0, 0.66u_1 + 0.4d_1 - 1 + s_3 = 0 \\
&-0.066u_1 - 0.4d_1 - 1 + s_4 = 0, u_1 - 1 \\
&+s_5 = 0, -u_1 - 1 + s_6 = 0 \\
&\sum_{j=1}^{6} \lambda_j = 1, \quad 1.41\lambda_1 - 1.41\lambda_2 + 0.66\lambda_3 \\
&-0.66\lambda_4 + \lambda_5 - \lambda_6 = 0, \sum_{j=1}^{6} z_j \le 2 \\
&\lambda_j - z_j \le 0, j = 1, \ldots, 6, s_j - U(1 - z_j) \le 0, \\
&j = 1, \ldots, 6, -\delta \le d_1 \le \delta \\
&z_j = \{0, 1\}, \quad \lambda_j, s_j \ge 0, j = 1, \ldots, 6 \qquad \text{(A1)}
\end{aligned}
$$

The equations defining the flexibility problem of the example in "High-Dimensional and Non-square Linear System: Dryer Control Problem" section are as follows:

$$
\begin{aligned}
&\mathrm{FI} = \min\ \delta \text{ s.t. } 9.0(u_1 - u_{1ss}) - 5.1(u_2 - u_{2ss}) - 0.8(u_3 - u_{3ss}) \\
&+ 0.31(u_4 - u_{4ss}) + 0.62(d_1 - d_{1ss}) + y_{1ss} - 1000 + s_1 = 0 \\
&-[9.0(u_1 - u_{1ss}) - 5.1(u_2 - u_{2ss}) - 0.8(u_3 - u_{3ss}) \\
&+ 0.31(u_4 - u_{4ss}) + 0.62(d_1 - d_{1ss}) + y_{1ss}] + 900 + s_2 = 0 \\
&0.06(u_1 - u_{1ss}) - 0.05(u_2 - u_{2ss}) + 0.03(u_3 - u_{3ss}) + y_{2ss} + s_3 = 0 \\
&-[0.06(u_1 - u_{1ss}) - 0.05(u_2 - u_{2ss}) + 0.03(u_3 - u_{3ss}) \\
&+y_{2ss}] - 4 + s_4 = 0, \quad 0.7(u_1 - u_{1ss}) - 0.4(u_2 - u_{2ss}) + y_{3ss} + 10 + s_5 = 0 \\
&-[0.7(u_1 - u_{1ss}) - 0.4(u_2 - u_{2ss}) + y_{3ss}] - 40 + s_6 = 0 \\
&-44.0(u_1 - u_{1ss}) - 3.0(u_2 - u_{2ss}) + 3.5(u_3 - u_{3ss}) \\
&+ 1.56(u_4 - u_{4ss}) - 1.1(d_1 - d_{1ss})(d_2 - d_{2ss}) + y_{4ss} - 170 + s_7 = 0 \\
&-[-44.0(u_1 - u_{1ss}) - 3.0(u_2 - u_{2ss}) + 3.5(u_3 - u_{3ss}) \\
&+ 1.56(u_4 - u_{4ss}) - 1.1(d_1 - d_{1ss})(d_2 - d_{2ss}) + y_{4ss}] + 100 + s_8 = 0 \\
&9.6(u_2 - u_{2ss}) - 1.5(d_1 - d_{1ss}) + y_{5ss} - 1650 + s_9 = 0 \\
&-[9.6(u_2 - u_{2ss}) - 1.5(d_1 - d_{1ss}) + y_{5ss}] - 1650 + s_{10} = 0 \\
&0.6(u_1 - u_{1ss}) - 0.03(u_3 - u_{3ss}) - 0.13(u_4 - u_{4ss}) \\
&+ 0.04(d_1 - d_{1ss}) + y_{6ss} - 1 + s_{11} = 0 \\
&-[0.6(u_1 - u_{1ss}) - 0.03(u_3 - u_{3ss}) - 0.13(u_4 - u_{4ss}) \\
&+ 0.04(d_1 - d_{1ss}) + y_{6ss}] + s_{12} = 0 \\
&u_1 - 95 + s_{13} = 0, \quad -u_1 + 30 + s_{14} = 0, \\
&u_2 - 95 + s_{15} = 0, \quad -u_2 + 40 + s_{16} = 0 \\
&u_3 - 100 + s_{17} = 0, \quad -u_3 + s_{18} = 0, \\
&u_4 - 90 + s_{19} = 0, \quad -u_4 + 20 + s_{20} = 0 \\
&\sum_{j=1}^{20} \lambda_j = 1, \quad \sum_{j=1}^{20} z_j \le 5 \\
&9.0\lambda_1 - 9.0\lambda_2 + 0.06\lambda_3 - 0.06\lambda_4 + 0.7\lambda_5 - 0.7\lambda_6 - 44.0\lambda_7 \\
&+ 44.0\lambda_8 + 0.6\lambda_{11} - 0.6\lambda_{12} + \lambda_{13} - \lambda_{14} = 0 \\
&-5.1\lambda_1 + 5.1\lambda_2 - 0.05\lambda_3 + 0.05\lambda_4 - 0.4\lambda_5 + 0.4\lambda_6 - 3.0\lambda_7 \\
&+ 3.0\lambda_8 + 9.6\lambda_9 - 9.6\lambda_{10} + \lambda_{15} - \lambda_{16} = 0
\end{aligned}
$$

$$
\begin{aligned}
&-0.8\lambda_1+0.8\lambda_2+0.03\lambda_3-0.03\lambda_4+3.5\lambda_7-3.5\lambda_8-0.03\lambda_{11}\\
&+\ 0.03\lambda_{12}+\lambda_{17}-\lambda_{18}=0\\
&0.31\lambda_1-0.31\lambda_2+1.56\lambda_7-1.56\lambda_8-0.13\lambda_{11}+0.13\lambda_{12}\\
&+\ \lambda_{19}-\lambda_{20}=0\\
&\lambda_j-z_j\le 0, j=1,\ldots,20, s_j-U(1-z_j)\le 0, j=1,\ldots,20\\
&50-20\delta\le d_1,\le 50+20\delta, -30\delta\le d_2\le 30\delta\\
&\quad z_j=\{0,1\},\quad \lambda_j,s_j\ge 0,\quad j=1,\ldots,20
\end{aligned}
\tag{A2}
$$

The equations defining the flexibility problem of the example in ''Steady-State Nonlinear Example: Shower Problem'' section are as follows:

$$
\begin{gathered}
\mathrm{FI}=\min\delta\ \text{s.t.}\quad (q_1-q_{1ss})+(q_2-q_{2ss})+F_{ss}-7+s_1=0,\\
-[(q_1-q_{1ss})+(q_2-q_{2ss})+F_{ss}]+3+s_2=0\ (q_1-q_{1ss})T_1\\
+(q_2-q_{2ss})(T_2-T_{2ss})+T_{ss}((q_1-q_{1ss})+(q_2-q_{2ss}))\\
-94((q_1-q_{1ss})+(q_2-q_{2ss}))+s_3=0\\
-[(q_1-q_{1ss})T_1+(q_2-q_{2ss})(T_2-T_{2ss})+T_{ss}((q_1-q_{1ss})\\
+\ (q_2-q_{2ss}))]+74((q_1-q_{1ss})+(q_2-q_{2ss}))+s_4=0\\
q_1-4.0+s_5=0,\ q_2-3.0+s_6=0,-q_1+s_7=0,q_2+s_8=0\\
\sum_{j=1}^{8}\lambda_j=1,\quad \sum_{j=1}^{8}z_j\le 3\\
\lambda_1-\lambda_2+\lambda_3(T_1+T_{ss}-94)+\lambda_4(-T_1-T_{ss}+74)+\lambda_5-\lambda_7=0\\
\lambda_1-\lambda_2+\lambda_3(T_1+T_{ss}-94)+\lambda_4(-T_1-T_{ss}+74)+\lambda_6-\lambda_8=0\\
\lambda_j-z_j\le 0, j=1,\ldots,8, s_j-U(1-z_j)\le 0, j=1,\ldots,8\\
120-10\delta\le T_2\le 120+10\delta,\ z_j=\{0,1\},\lambda_j,s_j\ge 0,j=1,\ldots,8
\end{gathered}
\tag{A3}
$$

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