I&EC research
Industrial & Engineering Chemistry Research
ARTICLE
pubs.acs.org/IECR

Two-Tier Search Strategy to Identify Nominal Operating Conditions for Maximum Flexibility

Vincentius Surya Kurnia Adi and Chuei-Tin Chang*

Department of Chemical Engineering, National Cheng Kung University, Tainan, Taiwan 70101, ROC

ABSTRACT: Traditionally, design and control issues have been addressed separately at different stages in the life cycle of a chemical plant. The process parameters are often selected in an ad hoc fashion during the design stage, and some of them later become the nominal set-point conditions in actual plant operation. The uncertain online disturbances associated with each set of operating conditions usually vary within a specific range centered at the nominal value. Because these arbitrarily chosen parameter values do not always result in the highest level of operational flexibility, it is thus desirable to develop a systematic method to optimally stipulate the nominal operating conditions of an existing process for maximum flexibility. The well-recognized flexibility index model is used in this work to evaluate system resiliency based on fixed nominal conditions, and a direct search method (differential evolution) is performed accordingly to identify the best candidates. Two examples are presented in this article to demonstrate the impacts of nominal settings and the effectiveness of the proposed optimization approach.

1. INTRODUCTION

The term "flexibility" is generally regarded as the capability of a system to function adequately under various sources of uncertainties.[1] It has also been recognized[2−5] that these uncertainties might be due to inaccuracies in the estimates of model parameters for design calculations (such as heat-transfer coefficients, reaction rate constants, and other physical properties) or external disturbances in process conditions during actual operations (such as the qualities and flow rates of feed streams). The latter conditions often fluctuate online within some statistically determinable ranges, whereas their nominal values can be stipulated and adjusted offline within definite lower and upper bounds that are physically tolerable by the system/equipment. Specific examples of such scenarios can be found in later sections of this article.

Traditionally, design and control decisions are made in sequential stages over the life cycle of a chemical plant. In the design phase, the "optimal" operating conditions and the corresponding material and energy balance data are determined mainly on the basis of economic considerations. In the subsequent step, the control systems are configured to maintain the key process conditions at the fixed nominal values. Because it is often desirable to address the operability issues at the earliest possible stage, the systematic incorporation of flexibility analysis in process synthesis and design has received considerable attention in recent years.[6−13] The so-called flexibility index (FI) was proposed by Swaney and Grossmann[12,13] to provide a quantitative measure of the feasible region in the parameter space. More specifically, the FI can be associated with the maximum allowable deviations of the uncertain parameters from their nominal values, under which feasible operation can be assured with proper manipulation of the control variables. A series of subsequent studies focused on improving and extending the use of this index in grassroots and revamp designs.[14−16] Although satisfactory results were reported, none of the studies considered the important problem of setting the most appropriate nominal conditions to maximize the FI.

The potential benefits of manipulating the nominal values of uncertain parameters are basically two-fold. First, the operational flexibility of a given chemical plant could be enhanced without extra capital investments. In addition, the operating cost of a system with higher flexibility is arguably lower because the system can cope with more extreme conditions without shutdown. Therefore, the main objective of this work is to develop an effective optimization strategy for identifying the best nominal conditions to maximize the flexibility index (FI).

According to Swaney and Grossmann,[13] the FI is usually determined in a minimization process on the basis of a mixed integer nonlinear programming (MINLP) model with fixed nominal parameter values. Consequently, a two-tier search algorithm is needed to solve the corresponding max−min optimization problem for the research objective mentioned above. A direct search method is adopted in the present study to perform maximization runs at the upper level, and the original flexibility index model is used at the lower level to carry out the well-established minimization computations. The main reason for selecting a direct search approach in this framework is the need to simplify the problem formulation by avoiding the use of gradients. One of the most popular multiagent direct search strategies is the so-called genetic algorithm (GA) (e.g., see Holland[17] and Goldberg[18]). There are also two other closely related optimization methods, namely, differential evolution[19,20] (DE) and particle swarm optimization[21−23] (PSO). DE is conceptually similar to GA in its use of evolutionary operators to guide the search toward an optimum, but it was specifically developed for real-valued search spaces from the start. PSO was originally intended as a model for the social behavior in a flock of birds, but the algorithm was later simplified for solving optimization problems. Earlier studies showed that DE fared best on a number of common benchmark problems,[24] and therefore, it was chosen as the direct search optimizer for the present study.

Received: May 17, 2011
Accepted: August 9, 2011
Revised: July 18, 2011
Published: August 09, 2011

Based on the above discussions, it is clear that the unique features of this work include

(a) a refined uncertainty concept that is characterized by the uncertain ranges in terms of both physical and statistical limits,
(b) a modified problem definition in which some of the nominal values of process parameters are allowed to be manipulated, and
(c) a two-tier search strategy that is developed by integrating the existing MINLP solver and a direct search method (i.e., DE) to solve the max−min optimization problem at hand.

The rest of the article is organized as follows: The problem statement is presented in the next section, which includes specifications of the basic assumptions, the given data, and the expected results. In section 3, the detailed formulation of the proposed dual-stage max−min mathematical programming model is provided. A two-tier search algorithm was developed in the present study for solving the proposed mathematical model, and this strategy is described in section 4. Two examples are given in section 5 to demonstrate the feasibility of the solution procedure and also the impacts of nominal settings on system flexibility. Finally, the conclusions of this work are drawn in section 6.

2. PROBLEM STATEMENT

Let us assume that, for a given system, the conventional flexibility index model[13] is available. Let us further assume that the set of uncertainty parameter nominal values, $\boldsymbol{\theta}^{\mathrm{N}}$, can be divided into two different types, that is

$$\boldsymbol{\theta}^{\mathrm{N}} = \begin{bmatrix} \boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}} \\ \boldsymbol{\theta}_{\mathrm{II}}^{\mathrm{N}} \end{bmatrix} \tag{1}$$

where the set $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ can be adjusted offline with existing equipment (e.g., feed quality and flow rate, removal ratio, etc.) whereas $\boldsymbol{\theta}_{\mathrm{II}}^{\mathrm{N}}$ is unalterable (e.g., heat-transfer coefficients, reaction rate constants, physical properties, etc.).

In addition, the initial estimates of the nominal values of both types of parameters are given. The search results of the proposed strategy should include (1) the maximum value of FI for the system considered and (2) the optimal nominal values of $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$.

3. MODEL FRAMEWORK

As mentioned previously, Swaney and Grossmann[12,13] developed the concept of the flexibility index, which is a single scalar measure of the allowable variations in all uncertain parameters. Although a thorough treatment of this issue has been provided by Biegler et al.,[25] the basic framework of the flexibility index model is briefly outlined here for illustration clarity and completeness. First, let us define the label sets for equality and inequality constraints

$$\mathbf{I} = \{i | i \text{ is the label of an equality constraint}\} \tag{2}$$

$$\mathbf{J} = \{j | j \text{ is the label of an inequality constraint}\} \tag{3}$$

The general design model can be expressed as

$$h_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0, \quad i \in \mathbf{I} \tag{4}$$

$$g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \le 0, \quad j \in \mathbf{J} \tag{5}$$

where h_i is the ith equality constraint in the design model (e.g., the mass balance equation for a processing unit), g_j is the jth inequality constraint in the design model (e.g., a capacity limit), $\mathbf{d}$ represents a vector in which all design variables are stored, $\mathbf{z}$ denotes the vector of adjustable control variables, $\mathbf{x}$ is the vector of state variables, and $\boldsymbol{\theta}$ denotes the vector of uncertain parameters. Notice that the uncertain parameters can also be divided into two groups according to eq 1. The parameter space, $\Gamma(\delta)$, can be expressed as

$$\Gamma(\delta) = \{\boldsymbol{\theta}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}^{-} \le \boldsymbol{\theta} \le \boldsymbol{\theta}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}^{+}\} \tag{6}$$

where $\Delta\boldsymbol{\theta}^{+}$ and $\Delta\boldsymbol{\theta}^{-}$ denote the vectors of expected deviations in the positive and negative directions, respectively, and $\delta \ge 0$ is a scalar variable. The flexibility index was traditionally regarded as the maximum value of δ that renders all points in $\Gamma(\delta)$ feasible.[10,11] This flexibility index can be determined by solving the nonconvex MINLP model

$$\mathrm{FI} = \min_{\delta, \boldsymbol{\mu}, \boldsymbol{\lambda}, \mathbf{s}, \mathbf{y}, \mathbf{x}, \mathbf{z}} \delta \tag{7}$$

subject to the constraints in eqs 4 and 8−17

$$g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) + s_j = 0, \quad j \in \mathbf{J} \tag{8}$$

$$\sum_{i \in \mathbf{I}} \mu_i \frac{\partial h_i}{\partial \mathbf{z}} + \sum_{j \in \mathbf{J}} \lambda_j \frac{\partial g_j}{\partial \mathbf{z}} = 0 \tag{9}$$

$$\sum_{i \in \mathbf{I}} \mu_i \frac{\partial h_i}{\partial \mathbf{x}} + \sum_{j \in \mathbf{J}} \lambda_j \frac{\partial g_j}{\partial \mathbf{x}} = 0 \tag{10}$$

$$\sum_{j \in \mathbf{J}} \lambda_j = 1 \tag{11}$$

$$\lambda_j - y_j \le 0, \quad j \in \mathbf{J} \tag{12}$$

$$s_j - Q(1 - y_j) \le 0, \quad j \in \mathbf{J} \tag{13}$$

$$\sum_{j \in \mathbf{J}} y_j = m + 1 \tag{14}$$

$$\boldsymbol{\theta}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}^{-} \le \boldsymbol{\theta} \le \boldsymbol{\theta}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}^{+} \tag{15}$$

$$y_j = \{0, 1\}, \quad \lambda_j \ge 0, \quad s_j \ge 0, \quad j \in \mathbf{J} \tag{16}$$

$$\delta \ge 0 \tag{17}$$

where s_j is the slack variable for the jth inequality constraint, Q denotes a large enough positive number to be used as the upper bound of s_j, μ_i denotes the Lagrange multiplier of equality constraint h_i, λ_j is the Lagrange multiplier of inequality constraint g_j, and y_j denotes the binary variable reflecting whether the corresponding inequality constraint is active (i.e., $g_j = 0$ if $y_j = 1$, whereas $g_j < 0$ if $y_j = 0$). Because the aforementioned model has been published extensively in the literature,[1,12,13] further details are omitted for the sake of brevity.

Notice that the conventional flexibility index model considers only *fixed* nominal parameter values. To find the optimal FI by varying the nominal operating conditions in $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$, a dual-level optimization procedure is needed, that is

$$\mathrm{FI}_{\max} = \max_{\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}} \min_{\delta, \boldsymbol{\mu}, \boldsymbol{\lambda}, \mathbf{s}, \mathbf{y}, \mathbf{x}, \mathbf{z}} \delta \tag{18}$$

Almost all constraints of this optimization problem should be the same as those used in the original flexibility index model, namely,

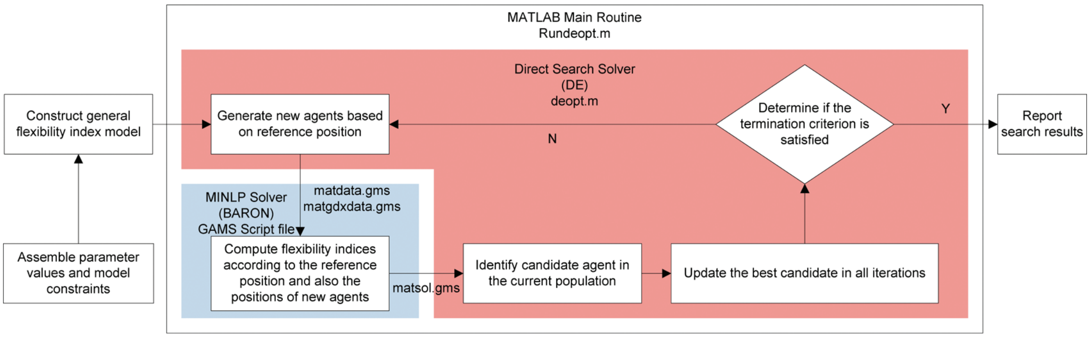

Figure 1. Two-tier search strategy.

eqs 4, 8−14, 16, and 17, whereas eq 15 should be replaced by

$$\begin{aligned} &\boldsymbol{\theta}_{\mathrm{I}}^{\min} \le \boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}_{\mathrm{I}}^{-} \le \boldsymbol{\theta}_{\mathrm{I}} \le \boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}_{\mathrm{I}}^{+} \le \boldsymbol{\theta}_{\mathrm{I}}^{\max} \\ &\boldsymbol{\theta}_{\mathrm{II}}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}_{\mathrm{II}}^{-} \le \boldsymbol{\theta}_{\mathrm{II}} \le \boldsymbol{\theta}_{\mathrm{II}}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}_{\mathrm{II}}^{+} \end{aligned} \tag{19}$$

where $\boldsymbol{\theta}_{\mathrm{I}}^{\min}$ and $\boldsymbol{\theta}_{\mathrm{I}}^{\max}$ represent the lower and upper limits, respectively, of realizable values of the type-I parameters. These limits are necessary because $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ should now be viewed as a vector of decision variables and, therefore, the corresponding parameter intervals, namely, $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}} - \delta\Delta\boldsymbol{\theta}_{\mathrm{I}}^{-} \le \boldsymbol{\theta}_{\mathrm{I}} \le \boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}} + \delta\Delta\boldsymbol{\theta}_{\mathrm{I}}^{+}$, are no longer bounded. Notice that $\Delta\boldsymbol{\theta}_{\mathrm{I}}^{-}$ and $\Delta\boldsymbol{\theta}_{\mathrm{I}}^{+}$ are used in the proposed model to characterize the ranges of statistically uncertain parameters, but $\boldsymbol{\theta}_{\mathrm{I}}^{\min}$ and $\boldsymbol{\theta}_{\mathrm{I}}^{\max}$ are needed for setting the lower and upper bounds that are physically tolerable by the system/equipment.

An often-used approach to facilitate transformation of eq 18 into a single-layer optimization framework is to convert the lower-level problem into a set of equality and inequality constraints by invoking the Karush−Kuhn−Tucker (KKT) conditions. However, it is clear from eqs 8−17 that integer variables are involved and, therefore, this approach is not really applicable. Because the explicit functional form of the FI in eq 7 (i.e., the lower-level optimum in eq 18) and its gradients cannot be obtained readily, a direct search strategy, namely, the differential evolution (DE) algorithm, is employed in this work to handle the upper-level maximization problem. Finally, it should be cautioned that any chosen search strategy inevitably suffers the curse of dimensionality.[24] In other words, as the dimension of $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ increases, the computation cost for implementing the proposed solution strategy might eventually become prohibitive.

4. TWO-TIER SEARCH STRATEGY

As mentioned previously, the optimization problem in eq 18 is tackled hierarchically on two levels. First, the MINLP formulated in eqs 4, 7−14, 16, 17, and 19 is solved to minimize δ based on a set of fixed nominal parameters in $\boldsymbol{\theta}^{\mathrm{N}}$, and then, on the second level, the maximum value of the flexibility index is determined by adjusting the nominal operating conditions in $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ according to DE algorithm. A DE optimizer basically creates the agent positions randomly on the basis of a reference position and then updates this reference position to improve its fitness or to minimize a cost function. A commonly used DE procedure was developed by Storn et al.,[19,20] and for the sake of completeness, a brief description is presented in Appendix A. The proposed two-tier search strategy can be concisely depicted with the flowchart in Figure 1. A brief explanation of each step in this procedure is provided as follows:

(1) *Assemble parameter values and model constraints.* Obtain all parameter values in the proposed model, including the initial estimates of $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$. Formulate all model constraints based on eqs 4, 8−14, 16, 17, and 19.

(2) *Construct computer codes for solving the generalized flexibility index model.* Build a GAMS code in a script file according to eqs 4, 7−14, 16, 17, and 19. The model parameters in $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ are allowed to be varied through the MATLAB−GAMS interface.[26]

(3) *Generate new agents based on reference position.* Use the best candidate as a reference to generate new agents with DE optimizer. The required computation process is explained in the Appendix A.

(4) *Compute flexibility indices according to the reference position and also the positions of new agents.* Execute the aforementioned GAMS code repeatedly with the BARON solver to determine a collection of flexibility indices using the reference parameter values in $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ and also those specified in the NP new agents.

(5) *Identify a candidate agent in the current population.* The agent yielding the highest FI value is picked from the population in the present iteration.

(6) *Update the best candidate in all iterations.* If the FI value of the current candidate is greater than that of the best candidate in the previous iteration, the current candidate is adopted to replace the old one. Otherwise, the current candidate is discarded.

(7) *Determine if the termination criterion is satisfied.* The iteration process is terminated when an assigned iteration number is reached or an adequate level of fitness is achieved, that is

$$-\boldsymbol{\varepsilon} \le \frac{\boldsymbol{\theta}_{\mathrm{I},k}^{\mathrm{N}} - \boldsymbol{\theta}_{\mathrm{I},k+1}^{\mathrm{N}}}{\boldsymbol{\theta}_{\mathrm{I},k}^{\mathrm{N}}} \le \boldsymbol{\varepsilon} \tag{20}$$

where $\boldsymbol{\varepsilon}$ is a vector of error bounds and k denotes iteration number.

(8) *Report the search results.* The search results are mainly the optimal $\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ and the corresponding FI.

5. EXAMPLES

Two examples are presented in this section to demonstrate the impacts of nominal settings on flexibility and the effectiveness of the proposed optimization approach. A dryer control problem, originally formulated by Lima et al.,[2−4] is first analyzed to illustrate the effectiveness of the proposed approach in realistic applications. A water network design problem is then considered, mainly because of the higher dimensionality of uncertainty parameters. Both problems were solved on a PC equipped with an Intel Core2 Quad CPU Q9400 and 4.00 GB RAM (3.25 GB usable) 32-bit operating system platform.

Table 1. Process variables Used for the Dryer Control Problem in Example 1

process variable	definition	units	lower bound	upper bound
MV1 (z_1)	gas flow SP	0−1 ratio	0.3	0.95
MV2 (z_2)	feed screw amps SP	0−1 ratio	0.4	0.95
MV3 (z_3)	secondary damper VP	0−1 ratio	0	1
MV4 (z_4)	scrubber orifice VP	0−1 ratio	0.2	0.9
CV1 (x_1)	inlet temperature	°C	900	1000
CV2 (x_2)	outlet temperature	°C	−4	0
CV3 (x_3)	combustion-chamber pressure	kPa_g	−40	−10
CV4 (x_4)	bag-house pressure	kPa_g	100	170
CV5 (x_5)	main fan hp	kW	1300	1650
CV6 (x_6)	predicted exit moisture	%	0	1
DV1 (θ_1)	mixer amps	A	30	70
DV2 (θ_2)	inlet moisture	%	0	60

The MINLP solver BARON in GAMS is utilized to carry out the lower-level optimization runs specified in step 4 of the proposed search procedure. The DE optimizer,[19,20] which is coded in script file deopt.m on the MATLAB platform, is used to generate new agent positions (step 3). An existing MATLAB−GAMS interface[28] has been modified to facilitate data transfer between these two levels. The values of type-I parameters are passed from MATLAB to GAMS using data files matdata.gms and matgdxdata.gms, and the GAMS output in matsol.gms is passed back to the MATLAB environment. Finally, all steps in the proposed search strategy are controlled and implemented according to Figure 1 with the main MATLAB routine rundeopt.m.

5.1. Example 1: Dryer Control Problem. Consider the flowsheet presented in Lima et al.[4] (see Figure 2). Basically, ambient air, heated by natural gas combustion, is mixed with a flow of wet particles. The mixture obtained is conveyed through a dryer/scrubber/bag house unit with an induction fan. The process is highly interactive and subject to internal flow and pressure disturbances due to caking of partially dried material on the sides of the dryer. The operation objective is to put as much material as possible through the unit subject to constraints on measurements characterizing temperature, pressure, and final particle moisture and to minimize natural gas consumption at the same time.

This process can be modeled by the following steady-state gain equations and constraining sets[2−4]

$$\begin{pmatrix} x_1 - x_1^{ss} \\ x_2 - x_2^{ss} \\ x_3 - x_3^{ss} \\ x_4 - x_4^{ss} \\ x_5 - x_5^{ss} \\ x_6 - x_6^{ss} \end{pmatrix} = \begin{pmatrix} 9.00 \\ 0.06 \\ 0.70 \\ -44.00 \\ 0 \\ 0.60 \end{pmatrix} \begin{pmatrix} 9.00 & -5.10 & -0.80 & 0.31 \\ 0.06 & -0.05 & 0.03 & 0 \\ 0.70 & -0.40 & 0 & 0 \\ -44.00 & -3.00 & 3.50 & 1.56 \\ 0 & 9.60 & 0 & 0 \\ 0.60 & 0 & -0.03 & -0.13 \end{pmatrix} \begin{pmatrix} z_1 - z_1^{ss} \\ z_2 - z_2^{ss} \\ z_3 - z_3^{ss} \\ z_4 - z_4^{ss} \end{pmatrix} + \begin{pmatrix} 0.62 & 0 \\ 0 & 0 \\ 0 & 0 \\ -1.10 & 1 \\ -1.50 & 0 \\ 0.04 & 0 \end{pmatrix} \begin{pmatrix} \theta_1 - \theta_1^{ss} \\ \theta_2 - \theta_2^{ss} \end{pmatrix} \tag{21}$$

and

$$\mathrm{DOS} = \left\{ \mathbf{x} \in \mathscr{R}^6 | 900 \le x_1 \le 1000, -4 \le x_2 \le 0, -40 \le x_3 \le -10, 100 \le x_4 \le 170, 1300 \le x_5 \le 1650, 0 \le x_6 \le 1 \right\}$$

$$\mathrm{AIS} = \{ \mathbf{z} \in \mathscr{R}^4 | 0.3 \le z_1 \le 0.95, 0.4 \le z_2 \le 0.95, 0 \le z_3 \le 1, 0.2 \le z_4 \le 0.9 \}$$

$$\mathrm{EDS} = \{ \boldsymbol{\theta} \in \mathscr{R}^2 | 30 \le \theta_1 \le 70, 0 \le \theta_2 \le 60 \} \tag{22}$$

where **x** denotes a vector of six controlled variables (CVs), **z** denotes a vector of four manipulated variables (MVs), and $\boldsymbol{\theta}$ is a vector of two disturbance variables (DVs). The definitions of these variables can be found in Table 1. The desired output set (DOS) is the desired ranges of outputs to be achieved, and the available input set (AIS) is the set of values that the process input variables can take. Finally, notice that the expected disturbance set (EDS) represents the expected steady-state values of the disturbances, and this set can be used to reflect uncertainties in model parameters.

It is assumed in this study that the steady-state values of controlled, manipulated, and disturbance variables are located at the midpoints of their respective ranges, that is, $\mathbf{x}^{ss} = (950.0\ -2.0\ -25.0\ 135.0\ 1475.0\ 0.5)^T$, $\mathbf{z}^{ss} = (0.625\ 0.675\ 0.5\ 0.55)^T$, and $\boldsymbol{\theta}^{ss} = (50.0\ 30.0)^T$. From the expected disturbance set EDS, one can see that $\Delta\theta_1^- = \Delta\theta_1^+ = 20$ and $\Delta\theta_2^- = \Delta\theta_2^+ = 30$. The flexibility index model can therefore be constructed according to eqs 21 and 22 and these reference points (see Appendix B). The corresponding FI of this system was found to be 0.944.

We next assume that all expected steady-state values in EDS are adjustable, that is, they can be categorized as $\boldsymbol{\theta}_I^N$, and their initial values are $\theta_1^N = \theta_1^{ss} = 50$ and $\theta_2^N = \theta_2^{ss} = 30$. Also, the realizable values of both parameters are assumed to be between 30 and 70 for θ_1^N and between 0 and 100 for θ_2^N. The proposed search strategy was utilized to locate the maximum FI. The corresponding convergence process of the negative values of FI can be found in Figure 3. Two alternative termination criteria are employed in the search procedure according to iteration number and relative error (defined in eq 20). For the current example, the maximum iteration number is set to 50, and all relative error bounds are set to 10^{-6}. A population size of 20 was found to be sufficient for obtaining good results, and a computational time of roughly 1000 s was needed to locate the optimal FI. The maximum FI identified in the search process is 0.97219 (+2.99%) and the corresponding values of θ_1^N and θ_2^N are 49.444 and 30.774, respectively. The DE agents were randomly spread within the aforementioned search range in the beginning (see Figure 4), and most of the agents eventually converged around the optimal value.

5.2. Example 2: Water Network Problem. The basic water network considered here consists of one primary source W1, one secondary source W2, one sink S1, two water-using units U1 and

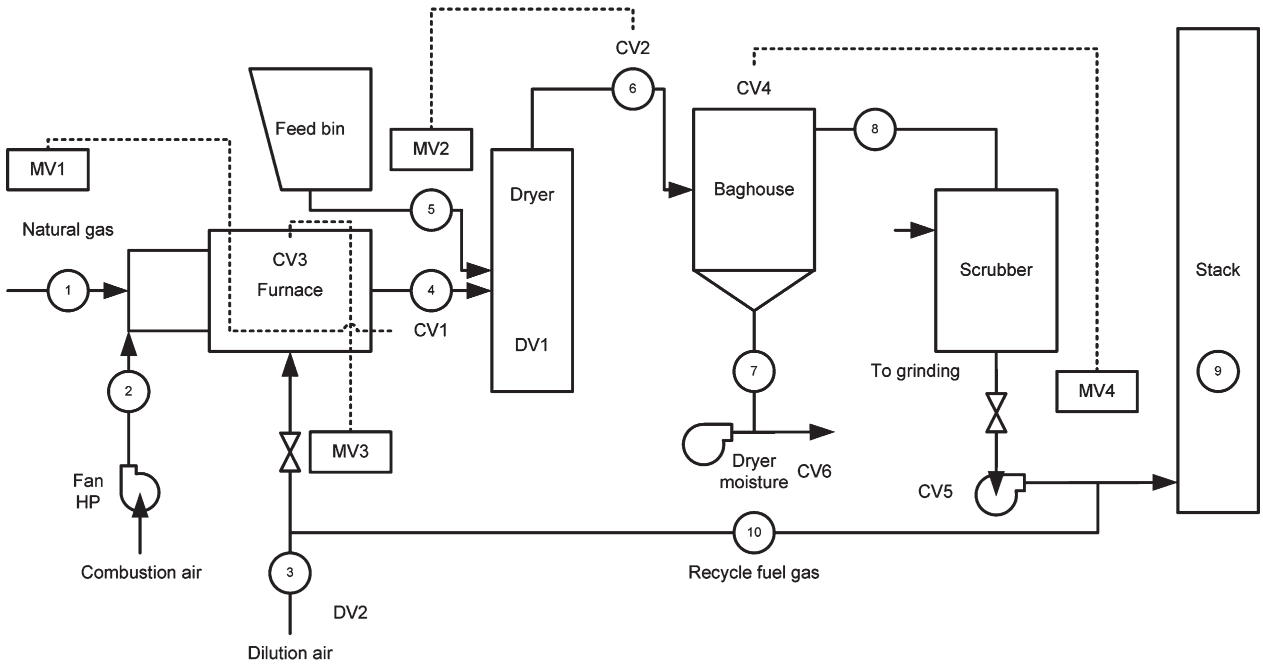

Figure 2. Process flow diagram for the dryer control problem in example 1.

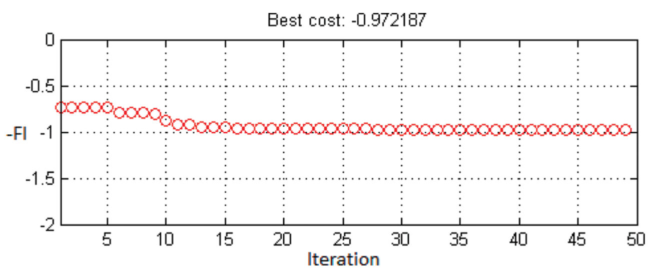

Figure 3. Iteration of the FI value obtained in example 1.

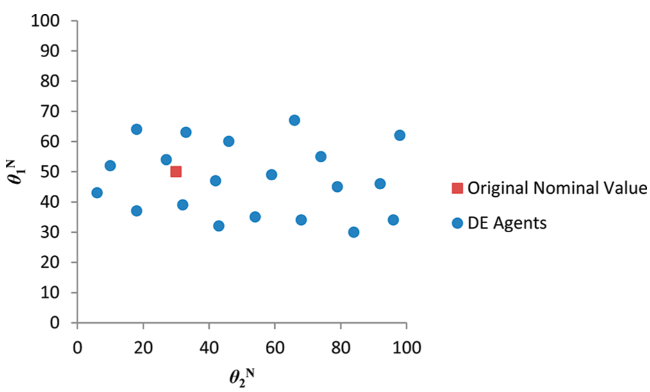

Figure 4. Initial agent positions in example 1.

U2, and a wastewater treatment unit T1 (see Figure 5). This structure was studied previously by Riyanto and Chang,[15] and the corresponding model parameters can be found in Table 2. Three uncertain parameters are considered in the present example, namely, the upper concentration limit of W2 (C_{w2}) and the mass loads of U1 and U2 (M_{u1} and M_{u2}). To characterize uncertainties more consistently, these parameters are normalized in the design model, that is

$$C_{w2} = \overline{C}_{w2}\theta_{C_{w2}} \tag{23}$$

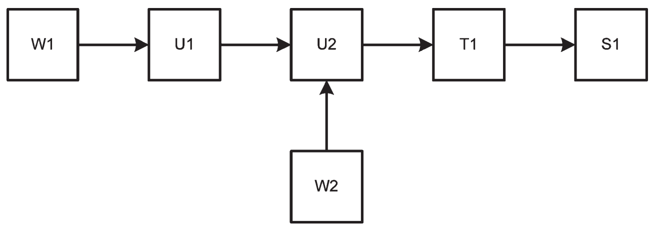

Figure 5. Basic structure of the water network.

Table 2. Model Parameters Used in the Water Network Problem

parameter	symbol	units	value
W1 maximum flow rate	F_{w1}^U	t/h	35000
W2 flow rate	F_{w2}	t/h	30000
W1 concentration	C_{w1}	ppm	0.100
W2 concentration	$\overline{C}_{w2}$	ppm	100000
U1 maximum inlet concentration	CI_{u1}^U	ppm	1
U2 maximum inlet concentration	CI_{u2}^U	ppm	80
T1 maximum inlet concentration	CI_{t1}^U	ppm	185
S1 maximum concentration	C_{s1}^U	ppm	30
U1 maximum outlet concentration	CO_{u1}^U	ppm	101
U2 maximum outlet concentration	CO_{u2}^U	ppm	240
T1 maximum flow rate	F_{t1}^U	t/h	125
U1 mass load	$\overline{M}_{u1}$	kg/h	2
U1 maximum tolerable mass load	M_{u1}^U	kg/h	4
U2 mass load	$\overline{M}_{u2}$	kg/h	5
U2 maximum tolerable mass load	M_{u2}^U	kg/h	8
T1 removal ratio	RR_{t1}		0.9

$$M_{u1} = \overline{M}_{u1}\theta_{M_{u1}} \tag{24}$$

$$M_{u2} = \overline{M}_{u2}\theta_{M_{u2}} \tag{25}$$

where $\overline{C}_{w2}$, $\overline{M}_{u1}$, and $\overline{M}_{u2}$ denote the reference parameter values and $\theta_{C_{w2}}$, $\theta_{M_{u1}}$, and $\theta_{M_{u2}}$ are the corresponding uncertain multipliers. The uncertain multipliers are assumed to be located within the parameter space defined by eq 6, in which all nominal levels are 1, that is

$$\theta^{N}_{C_{w2}} = \theta^{N}_{M_{u1}} = \theta^{N}_{M_{u2}} = 1 \tag{26}$$

and all corresponding positive and negative deviations equal 0.2, that is

$$\Delta\theta^{-}_{C_{w2}} = \Delta\theta^{+}_{C_{w2}} = \Delta\theta^{-}_{M_{u1}} = \Delta\theta^{+}_{M_{u1}} = \Delta\theta^{-}_{M_{u2}} = \Delta\theta^{+}_{M_{u2}} = 0.2 \tag{27}$$

By solving the conventional flexibility index model with fixed nominal conditions (see Appendix C), the maximum FI can be found to be 0.196. The only active constraint in this solution is associated with the maximum concentration at the inlet of U2 (CI^{U}_{u2}).

In this example, the nominal mass loads of both water-using units are assumed to be adjustable, and the corresponding multipliers (i.e., $\theta_{M_{u1}}$ and $\theta_{M_{u2}}$) can thus be regarded as type-I parameters in $\boldsymbol{\theta}_{I}$. Consequently, the only remaining multiplier, $\theta_{C_{w2}}$, should be treated as an uncertain parameter in $\boldsymbol{\theta}_{II}$. The DE optimizer was used to search for the largest possible FI of the given water network structure. Notice that, on the basis of eq 19, the agent positions should be distributed within a region that is bounded by the lower and upper limits of realizable type-I parameters. In the present case, this region is

$$\begin{aligned} 0 &\le \theta_{M_{u1}} \le \left(\frac{M^{U}_{u1}}{\bar{M}_{u1}}\right) \\ 0 &\le \theta_{M_{u2}} \le \left(\frac{M^{U}_{u2}}{\bar{M}_{u2}}\right) \end{aligned} \tag{28}$$

For the problem at hand, the maximum allowable number of iteration steps in the search process was set to 20, and every allowable upper limit of relative error was 10^{-6}. The initial population size was 5, and it took approximately 100 s to produce the optimal FI (1.6148). The corresponding convergence process can be found in Figure 6. According to the optimal solution, it can also be observed that the nominal values of $\theta^{N}_{M_{u1}}$ and $\theta^{N}_{M_{u2}}$ should be adjusted to 0.328 and 1.042, respectively. In other words, the nominal mass load of U1 needs to be reduced to about 32.8% of the original level (or 0.656 kg/h), whereas that of U2 should be 4.2% higher (i.e., 5.21 kg/h). This is clearly reasonable because the active constraint in the optimal solution of the original flexibility index model is associated with the maximum inlet concentration of U2.

Riyanto[27] suggested that, to improve the operational flexibility of a given water network, one can (1) raise the upper limit of freshwater supply rate and/or (2) modify the network structure. Although successful applications were reported, it should be noted that both approaches inevitably incur extra operating and/or capital costs. Additional cases are thus considered below to demonstrate the advantages of the present strategy.

Notice first that FI can be improved to 0.995 by raising the freshwater supply limit to 45 t/h. However, other than the extra freshwater cost, this improvement is obviously less impressive when compared with the FI value achieved by changing the nominal values (1.6148). Next consider a revamped structure proposed by Riyanto[27] (see Figure 7). Notice that a new pipeline is added from T1 to U2 to relax the active constraint corresponding to CI^{U}_{u2}. By solving the conventional flexibility index model with fixed nominal conditions, it can be found that such a revamped design improves FI to 3.829. In addition, the FI can be further raised to 4.226 by increasing the freshwater supply limit to 45 t/h for this revamped network. It can be observed that the corresponding active constraints are associated with the maximum inlet concentration of U2

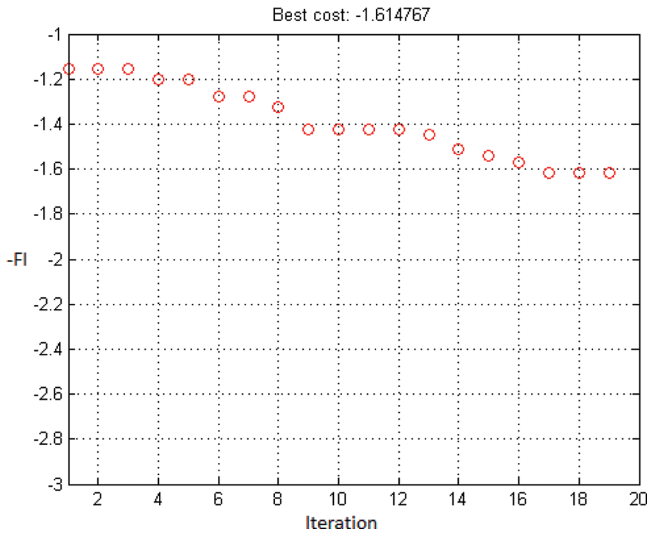

Figure 6. Iteration of the FI value obtained in example 2.

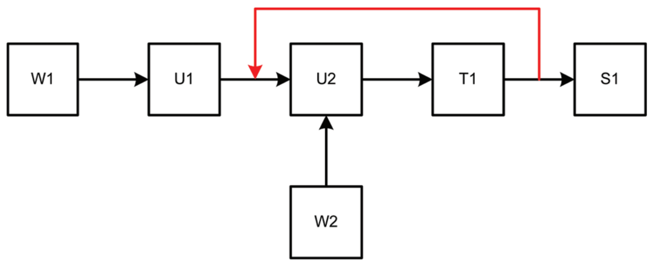

Figure 7. Revamped water network structure.

(CI^{U}_{u2}) and the maximum throughput of T1 (F^{U}_{t1}). It should again be noted that the aforementioned improvements can be realized only with additional operating/capital costs. Finally, further enhancement in operational flexibility can be achieved by changing the nominal values of $\theta^{N}_{M_{u1}}$ and $\theta^{N}_{M_{u2}}$ to 0.89096 and 0.91773, respectively. In particular, the FI can be raised to 4.452 without additional investments. These adjustments are obviously quite effective for relaxing the active constraints mentioned above.

6. CONCLUSIONS

The nominal parameter values arbitrarily selected in the design stage might result in a low level of system resiliency in actual plant operation. The possibility and benefits of adjusting nominal operating conditions to improve flexibility are clearly demonstrated in this article. A two-tier search strategy is also developed to solve the proposed max−min optimization problems. Two examples are provided to illustrate these promising ideas. Based on the case studies performed in this work, it can be observed that the impact of adjusting the nominal values of uncertainty parameters can be quite significant and should be considered as an additional means for enhancing the operational flexibility of any given system.

APPENDIX A: DIFFERENTIAL EVOLUTION ALGORITHM AND TUNING PARAMETERS

The DE algorithm works by generating several solution candidates (called agents). These agents are spread throughout the search-space according to simple mathematical formulas to calculate the coordinate of agents from the aforementioned population. If the new agent position has an improvement, then it is accepted and regarded as part of the population; otherwise, the new position is simply discarded. The process is iterated several times until a satisfactory solution is eventually found.

Let f: $\mathscr{R}^n \to \mathscr{R}$ be the fitness or minimized cost function. Every candidate solution is regarded as an argument to the function in the form of a vector of real numbers, and the given candidate solution produces a real number as output that indicates its fitness. The f gradient is not known. It is necessary to find a solution $\mathbf{m}$ for which $f(\mathbf{m}) \le f(\mathbf{p})$ for all $\mathbf{p}$ in the search space, which would mean that $\mathbf{m}$ is the global minimum. The function $h = -f$ can be considered for maximization of such a procedure.

Let $\mathbf{x} \in \mathscr{R}^n$ assign a candidate solution (agent) in the population. The basic DE algorithm can then be described as follows:

- Initialize all agents $\mathbf{x}$ randomly in the search space.
- Until a termination criterion is met (e.g., number of iterations performed, or adequate fitness reached), repeat the following:
  - For each agent $\mathbf{x}$ in the population, do the following:
    - Pick NP agents from the population at random such that all agents are different from each other as well as from agent $\mathbf{x}$.
    - Pick a random index $R \in \{1, ..., n\}$, where the highest possible value n is the dimensionality of the problem to be optimized.
    - Compute the agent's potentially new position $\mathbf{y} \in [y_1, ..., y_n]$ by iterating over each $I \in \{1, ..., n\}$ as follows:
      - Pick $r_i \sim U(0, 1)$ uniformly from the open range $(0, 1)$.
      - If $(i = R)$ or $(r_i < \mathrm{CR})$, let $y_i = a_i + F(b_i - c_i)$; otherwise, let $y_i = x_i$.
    - If $f(\mathbf{y}) < f(\mathbf{x})$, then replace the agent in the population with the improved candidate solution, that is, set $\mathbf{x} = \mathbf{y}$ in the population.
- Pick the agent from the population that has the lowest fitness and report it as the best found candidate solution of the corresponding iteration.

Notably, $F \in [0, 2]$ is called the differential weight, and $\mathrm{CR} \in [0, 1]$ is called the crossover probability; both of these parameters can be adjusted by the user along with the population size NP, where NP denotes the number of agents in the population. For the DE method, a standard choice of allegedly good behavioral parameters is found in the works by Storn et al.[17] and Liu and Lampinen,[28] which is a choice that also satisfies the theoretical conditions derived by Zaharie.[29] The DE parameters are not difficult to choose to obtain good results.[17] It is suggested that one use NP = 300 to obtain good results, and $F = 0.5$ is usually a good initial choice. If the population converges prematurely, then F should be increased. Values of F smaller than 0.4, like those greater than 1, are only occasionally effective. A good first choice for CR is 0.1, but because a large CR often speeds convergence, one should first try CR = 0.9 or CR = 1.0 to determine whether a quick solution is possible. For fastest convergence, it is best to pick the initial parameter range ($\mathscr{R}^n$) such that it covers the region of the suspected global optimum, although this choice does not seem to be mandatory.

APPENDIX B: CONVENTIONAL FLEXIBILITY INDEX MODEL FOR DRYER CONTROL PROBLEM

$$\mathrm{FI} = \min \delta$$

s.t.

$$9.0(z_1 - z_1^{ss}) - 5.1(z_2 - z_2^{ss}) - 0.8(z_3 - z_3^{ss}) + 0.31(z_4 - z_4^{ss}) + 0.62(\theta_1 - \theta_1^{ss}) + x_1^{ss} - 1000 + s_1 = 0$$

$$-[9.0(z_1 - z_1^{ss}) - 5.1(z_2 - z_2^{ss}) - 0.8(z_3 - z_3^{ss}) + 0.31(z_4 - z_4^{ss}) + 0.62(\theta_1 - \theta_1^{ss}) + x_1^{ss}] + 900 + s_2 = 0$$

$$-[9.0(z_1 - z_1^{ss}) - 5.1(z_2 - z_2^{ss}) - 0.8(z_3 - z_3^{ss}) + 0.31(z_4 - z_4^{ss}) + 0.62(\theta_1 - \theta_1^{ss}) + x_1^{ss}] + 900 + s_2 = 0$$

$$-[0.06(z_1 - z_1^{ss}) - 0.05(z_2 - z_2^{ss}) + 0.03(z_3 - z_3^{ss}) + x_2^{ss}] - 4 + s_4 = 0$$

$$0.7(z_1 - z_1^{ss}) - 0.4(z_2 - z_2^{ss}) + x_3^{ss} + 10 + s_5 = 0$$

$$-[0.7(z_1 - z_1^{ss}) - 0.4(z_2 - z_2^{ss}) + x_3^{ss}] - 40 + s_6 = 0$$

$$-44.0(z_1 - z_1^{ss}) - 3.0(z_2 - z_2^{ss}) + 3.5(z_3 - z_3^{ss}) + 1.56(z_4 - z_4^{ss}) - 1.1(\theta_1 - \theta_1^{ss})(\theta_2 - \theta_2^{ss}) + x_4^{ss} - 170 + s_7 = 0$$

$$-[-44.0(z_1 - z_1^{ss}) - 3.0(z_2 - z_2^{ss}) + 3.5(z_3 - z_3^{ss}) + 1.56(z_4 - z_4^{ss}) - 1.1(\theta_1 - \theta_1^{ss})(\theta_2 - \theta_2^{ss}) + x_4^{ss}] + 100 + s_8 = 0$$

$$9.6(z_2 - z_2^{ss}) - 1.5(\theta_1 - \theta_1^{ss}) + x_5^{ss} - 1650 + s_9 = 0$$

$$-[9.6(z_2 - z_2^{ss}) - 1.5(\theta_1 - \theta_1^{ss}) + x_5^{ss}] + 1300 + s_{10} = 0$$

$$0.6(z_1 - z_1^{ss}) - 0.03(z_3 - z_3^{ss}) - 0.13(z_4 - z_4^{ss}) + 0.04(\theta_1 - \theta_1^{ss}) + x_6^{ss} - 1 + s_{11} = 0$$

$$-[0.6(z_1 - z_1^{ss}) - 0.03(z_3 - z_3^{ss}) - 0.13(z_4 - z_4^{ss}) + 0.04(\theta_1 - \theta_1^{ss}) + x_6^{ss}] + s_{12} = 0$$

$$z_1 - 0.95 + s_{13} = 0, \quad -z_1 + 0.30 + s_{14} = 0, \quad z_2 - 0.95 + s_{15} = 0, \quad -z_2 + 0.40 + s_{16} = 0$$

$$z_3 - 1 + s_{17} = 0, \quad -z_3 + s_{18} = 0, \quad z_4 - 0.90 + s_{19} = 0, \quad -z_4 + 0.20 + s_{20} = 0$$

$$\sum_{j=1}^{20} \lambda_j = 1, \quad \sum_{j=1}^{20} y_j \le 5$$

$$9.0\lambda_1 - 9.0\lambda_2 + 0.06\lambda_3 - 0.06\lambda_4 + 0.7\lambda_5 - 0.7\lambda_6 - 44.0\lambda_7 + 44.0\lambda_8 + 0.6\lambda_{11} - 0.6\lambda_{12} + \lambda_{13} - \lambda_{14} = 0$$

$$-5.1\lambda_1 + 5.1\lambda_2 - 0.05\lambda_3 + 0.05\lambda_4 - 0.4\lambda_5 + 0.4\lambda_6 - 3.0\lambda_7 + 3.0\lambda_8 + 9.6\lambda_9 - 9.6\lambda_{10} + \lambda_{15} - \lambda_{16} = 0$$

$$-0.8\lambda_1 + 0.8\lambda_2 + 0.03\lambda_3 + 0.03\lambda_4 + 3.5\lambda_7 + 3.5\lambda_8 - 0.03\lambda_{11} + 0.03\lambda_{12} + \lambda_{17} - \lambda_{18} = 0$$

$$0.31\lambda_1 - 0.31\lambda_2 + 1.56\lambda_7 - 1.56\lambda_8 - 0.13\lambda_{11} + 0.13\lambda_{12} + \lambda_{19} - \lambda_{20} = 0$$

$$\lambda_j - y_j \le 0, \quad s_j = U(1 - y_j) \le 0, \quad j = 1, \; ... \; , 20$$

$$0 \le 50 - 20\delta \le \theta_1 \le 50 + 20\delta \le 70$$

$$0 \le 30 - 30\delta \le \theta_2 \le 30 + 30\delta \le 100$$

$$y_j = \{0, 1\}, \quad s_j \ge 0, \quad j = 1, \; ..., 20$$

 dx.doi.org/10.1021/ie201050w | Ind. Eng. Chem. Res. 2011, 50, 10707–10716

APPENDIX C: CONVENTIONAL FLEXIBILITY INDEX MODEL FOR WATER NETWORK PROBLEM

$$
\begin{aligned}
&\mathrm{FI} = \min \delta \\
&\text{s.t.} \\
&F_{w1} - f_{w1,u1} = 0\ (\mathrm{WB}_{w1}), \quad F_{w2} - f_{w2,u2} = 0\ (\mathrm{WB}_{w2}), \quad F_{s1} - f_{t1,s1} = 0\ (\mathrm{WB}_{s1}) \\
&F_{u1} - f_{w1,u1} = 0\ (\mathrm{WB}^{in}_{u1}), \quad F_{u2} - f_{w2,u2} - f_{u1,u2} - f_{t1,u2} = 0\ (\mathrm{WB}^{in}_{u2}), \quad F_{t1} - f_{u2,t1} = 0\ (\mathrm{WB}^{in}_{t1}) \\
&F_{u1} - f_{u1,u2} = 0\ (\mathrm{WB}^{out}_{u1}), \quad F_{u2} - f_{u2,t1} = 0\ (\mathrm{WB}^{out}_{u2}), \quad F_{t1} - f_{t1,u2} - f_{t1,s1} = 0\ (\mathrm{WB}^{out}_{t1}) \\
&F_{u1}\mathrm{CI}_{u1} - f_{w1,u1}C_{w1} = 0\ (\mathrm{CB}_{u1}), \quad F_{u2}\mathrm{CI}_{u2} - f_{w2,u2}\bar{C}_{w2}\theta_{C_{w2}} - f_{u1,u2}\mathrm{CO}_{u1} - f_{t1,u2}\mathrm{CO}_{t1} = 0\ (\mathrm{CB}_{u2}) \\
&F_{t1}\mathrm{CI}_{t1} - f_{u2,t1}\mathrm{CO}_{u2} = 0\ (\mathrm{CB}_{t1}), \quad F_{s1}C_{s1} - f_{t1,s1}\mathrm{CO}_{t1} = 0\ (\mathrm{CB}_{s1}) \\
&F_{u1}(\mathrm{CI}_{u1} - \mathrm{CO}_{u1}) + \bar{M}_{u1}\theta_{M_{u1}} = 0\ (\mathrm{PC}_{u1}), \quad F_{u2}(\mathrm{CI}_{u2} - \mathrm{CO}_{u2}) + \bar{M}_{u2}\theta_{M_{u2}} = 0\ (\mathrm{PC}_{u2}), \quad \mathrm{CI}_{t1}(1 - \mathrm{RR}_{t1}) - \mathrm{CO}_{t1} = 0\ (\mathrm{PC}_{t1}) \\
&F_{w1} - F^{U}_{w1} \le 0, \quad \mathrm{CI}_{u1} - \mathrm{CI}^{U}_{u1} \le 0, \quad \mathrm{CI}_{u2} - \mathrm{CI}^{U}_{u2} \le 0, \quad \mathrm{CO}_{u1} - \mathrm{CO}^{U}_{u1} \le 0 \\
&\mathrm{CO}_{u2} - \mathrm{CO}^{U}_{u2} \le 0, \quad \mathrm{CI}_{t1} - \mathrm{CI}^{U}_{t1} \le 0, \quad F_{t1} - F^{U}_{t1} \le 0, \quad C_{s1} - C^{U}_{s1} \le 0 \\
&\lambda_{F^U_{w1}} - y_{F^U_{w1}} \le 0, \quad \lambda_{\mathrm{CI}^U_{u1}} - y_{\mathrm{CI}^U_{u1}} \le 0, \quad \lambda_{\mathrm{CI}^U_{u2}} - y_{\mathrm{CI}^U_{u2}} \le 0, \quad \lambda_{\mathrm{CO}^U_{u1}} - y_{\mathrm{CO}^U_{u1}} \le 0 \\
&\lambda_{\mathrm{CO}^U_{u2}} - y_{\mathrm{CO}^U_{u2}} \le 0, \quad \lambda_{\mathrm{CI}^U_{t1}} - y_{\mathrm{CI}^U_{t1}} \le 0, \quad \lambda_{F^U_{t1}} - y_{F^U_{t1}} \le 0, \quad \lambda_{C^U_{s1}} - y_{C^U_{s1}} \le 0 \\
&\lambda_{F^U_{w1}} + \lambda_{\mathrm{CI}^U_{u1}} + \lambda_{\mathrm{CI}^U_{u2}} + \lambda_{\mathrm{CO}^U_{u1}} + \lambda_{\mathrm{CO}^U_{u2}} + \lambda_{\mathrm{CI}^U_{t1}} + \lambda_{F^U_{t1}} + \lambda_{C^U_{s1}} = 1 \\
&y_{F^U_{w1}} + y_{\mathrm{CI}^U_{u1}} + y_{\mathrm{CI}^U_{u2}} + y_{\mathrm{CO}^U_{u1}} + y_{\mathrm{CO}^U_{u2}} + y_{\mathrm{CI}^U_{t1}} + y_{F^U_{t1}} + y_{C^U_{s1}} \le 3 \\
&s_{F^U_{w1}} - U(1 - y_{F^U_{w1}}) \le 0, \quad s_{\mathrm{CI}^U_{u1}} - U(1 - y_{\mathrm{CI}^U_{u1}}) \le 0, \quad s_{\mathrm{CI}^U_{u2}} - U(1 - y_{\mathrm{CI}^U_{u2}}) \le 0, \quad s_{\mathrm{CO}^U_{u1}} - U(1 - y_{\mathrm{CO}^U_{u1}}) \le 0 \\
&s_{\mathrm{CO}^U_{u2}} - U(1 - y_{\mathrm{CO}^U_{u2}}) \le 0, \quad s_{\mathrm{CI}^U_{t1}} - U(1 - y_{\mathrm{CI}^U_{t1}}) \le 0, \quad s_{F^U_{t1}} - U(1 - y_{F^U_{t1}}) \le 0, \quad s_{C^U_{s1}} - U(1 - y_{C^U_{s1}}) \le 0 \\
&\mu_{\mathrm{WB}_{w1}} + \lambda_{F^U_{w1}} = 0, \quad -\mu_{\mathrm{WB}_{w1}} - \mu_{\mathrm{WB}^{in}_{u1}} - C_{w1}\mu_{\mathrm{CB}_{u1}} = 0, \quad -\mu_{\mathrm{WB}_{w2}} - \mu_{\mathrm{WB}^{in}_{u2}} - \bar{C}_{w2}\theta_{C_{w2}}\mu_{\mathrm{CB}_{u2}} = 0 \\
&\mu_{\mathrm{WB}^{in}_{u1}} + \mu_{\mathrm{WB}^{out}_{u1}} + \mathrm{CI}_{u1}\mu_{\mathrm{CB}_{u1}} + (\mathrm{CI}_{u1} - \mathrm{CO}_{u1})\mu_{\mathrm{PC}_{u1}} = 0 \\
&\mu_{\mathrm{WB}^{in}_{u2}} + \mu_{\mathrm{WB}^{out}_{u2}} + \mathrm{CI}_{u2}\mu_{\mathrm{CB}_{u2}} + (\mathrm{CI}_{u2} - \mathrm{CO}_{u2})\mu_{\mathrm{PC}_{u2}} = 0 \\
&\mu_{\mathrm{WB}^{in}_{t1}} + \mu_{\mathrm{WB}^{out}_{t1}} + \mathrm{CI}_{t1}\mu_{\mathrm{CB}_{t1}} + \lambda_{F^U_{t1}} = 0, \quad -\mu_{\mathrm{WB}^{in}_{u2}} - \mu_{\mathrm{WB}^{out}_{u2}} + \mathrm{CO}_{u1}\mu_{\mathrm{CB}_{u2}} = 0 \\
&-\mu_{\mathrm{WB}^{in}_{u2}} - \mu_{\mathrm{WB}^{out}_{u2}} + \mathrm{CO}_{t1}\mu_{\mathrm{CB}_{u2}} + \mu_{f_{t1,u2}} = 0, \quad -\mu_{\mathrm{WB}^{in}_{t1}} - \mu_{\mathrm{WB}^{out}_{u2}} + \mathrm{CO}_{u2}\mu_{\mathrm{CB}_{t1}} = 0 \\
&-\mu_{\mathrm{WB}^{out}_{t1}} - \mu_{\mathrm{WB}_{s1}} + \mathrm{CO}_{t1}\mu_{\mathrm{CB}_{s1}} = 0, \quad F_{u1}\mu_{\mathrm{CB}_{u1}} + F_{u1}\mu_{\mathrm{PC}_{u1}} + \lambda_{\mathrm{CI}^U_{u1}} = 0 \\
&F_{u2}\mu_{\mathrm{CB}_{u2}} + F_{u2}\mu_{\mathrm{PC}_{u2}} + \lambda_{\mathrm{CI}^U_{u2}} = 0, \quad F_{t1}\mu_{\mathrm{CB}_{t1}} + (1 - \mathrm{RR}_{t1})\mu_{\mathrm{PC}_{t1}} + y_{\mathrm{CI}^U_{t1}} = 0 \\
&-f_{u1,u2}\mu_{\mathrm{CB}_{u2}} - F_{u1}\mu_{\mathrm{PC}_{u1}} + y_{\mathrm{CO}^U_{u1}} = 0, \quad -f_{u2,t1}\mu_{\mathrm{CB}_{t1}} - F_{u2}\mu_{\mathrm{PC}_{u2}} + y_{\mathrm{CO}^U_{u2}} = 0 \\
&-f_{t1,s1}\mu_{\mathrm{CB}_{s1}} - \mu_{\mathrm{PC}_{t1}} = 0, \quad \mu_{\mathrm{WB}_{s1}} + C_{s1}\mu_{\mathrm{CB}_{s1}} = 0, \quad F_{s1}\mu_{\mathrm{CB}_{s1}} + \lambda_{C^U_{s1}} = 0 \\
&0 \le 1 - 0.2\delta \le \theta_{C_{w2}} \le 1 + 0.2\delta \\
&0 \le \theta^{N}_{M_{u1}} - 0.2\delta \le \theta_{M_{u1}} \le \theta^{N}_{M_{u1}} + 0.2\delta \le \left(\frac{M^{U}_{u1}}{\bar{M}_{u1}}\right) \\
&0 \le \theta^{N}_{M_{u2}} - 0.2\delta \le \theta_{M_{u2}} \le \theta^{N}_{M_{u2}} + 0.2\delta \le \left(\frac{M^{U}_{u2}}{\bar{M}_{u2}}\right) \\
&y_{F^U_{w1}}, y_{\mathrm{CI}^U_{u1}}, y_{\mathrm{CI}^U_{u2}}, y_{\mathrm{CO}^U_{u1}}, y_{\mathrm{CO}^U_{u2}}, y_{\mathrm{CI}^U_{t1}}, y_{F^U_{t1}}, y_{C^U_{s1}} \in \{0, 1\} \\
&s_{F^U_{w1}}, s_{\mathrm{CI}^U_{u1}}, s_{\mathrm{CI}^U_{u2}}, s_{\mathrm{CO}^U_{u1}}, s_{\mathrm{CO}^U_{u2}}, s_{\mathrm{CI}^U_{t1}}, s_{F^U_{t1}}, s_{C^U_{s1}} \ge 0
\end{aligned}
$$

AUTHOR INFORMATION

Corresponding Author

*E-mail: ctchang@mail.ncku.edu.tw.

ACKNOWLEDGMENT

The authors thank the National Science Council of Taiwan for supporting this research under Grant NSC 98-2621-M-006-006.

NOMENCLATURE

Acronyms

AIS = available input set
CB = component balance
CV = controlled variable
DE = differential evolution
DOS = desired output set
DV = disturbance variable
EDS = expected disturbance set
FI = flexibility index
GA = genetic algorithm
KKT = Karush−Kuhn−Tucker
MINLP = mixed integer nonlinear programming
MV = manipulated variable
PC = performance characterization

PSO = particle swarm optimization
WB = water balance

Variables

C = overall concentration of the specific unit
CI = inlet concentration of the specific unit
CO = outlet concentration of the specific unit
$\mathbf{d}$ = vector of design variables
F = total flow rate
f = specific branch flow rate
FI_{max} = optimal FI
g_j = inequality constraints
h_i = equality constraints
$\mathbf{I}$ = set of equality constraints
$\mathbf{J}$ = set of inequality constraints
k = iteration number
M = mass load of the specific water-using unit
$\overline{M}$ = mass load nominal value of the specific water-using unit
m = number of control variables
$\mathcal{R}$ = real number set
RR = removal ratio of water treatment unit
s_j = slack variable for the jth inequality constraint
U = big real value
$\mathbf{x}$ = vector of state variables
y_j = binary variables reflecting the active jth inequality constraint
$\mathbf{z}$ = vector of control variables

Greek Letters

$\Gamma(\delta)$ = parameter space of δ
δ = deviation due to uncertainties
$\Delta\boldsymbol{\theta}^+$ = expected deviations of uncertainties, positive direction
$\Delta\boldsymbol{\theta}^-$ = expected deviations of uncertainties, negative direction
$\Delta\boldsymbol{\theta}_{\mathrm{I}}^+$ = expected deviations of $\boldsymbol{\theta}_{\mathrm{I}}$, positive direction
$\Delta\boldsymbol{\theta}_{\mathrm{I}}^-$ = expected deviations of $\boldsymbol{\theta}_{\mathrm{I}}$, negative direction
$\Delta\boldsymbol{\theta}_{\mathrm{II}}^+$ = expected deviations of $\boldsymbol{\theta}_{\mathrm{II}}$, positive direction
$\Delta\boldsymbol{\theta}_{\mathrm{II}}^-$ = expected deviations of $\boldsymbol{\theta}_{\mathrm{II}}$, negative direction
$\boldsymbol{\theta}^{\mathrm{N}}$ = set of uncertainty parameter nominal values
$\boldsymbol{\theta}_{\mathrm{I}}^{\mathrm{N}}$ = set of alterable offline uncertainty parameter nominal values
$\boldsymbol{\theta}_{\mathrm{II}}^{\mathrm{N}}$ = set of unalterable uncertainty parameter nominal values
$\boldsymbol{\theta}$ = vector of uncertain parameters
$\boldsymbol{\theta}_{\mathrm{I}}$ = vector of alterable offline uncertainty parameters
$\boldsymbol{\theta}_{\mathrm{II}}$ = vector of unalterable uncertainty parameters
$\boldsymbol{\theta}_{\mathrm{I}}^{\max}$ = physical system upper limit of $\boldsymbol{\theta}_{\mathrm{I}}$
$\boldsymbol{\theta}_{\mathrm{I}}^{\min}$ = physical system lower limit of $\boldsymbol{\theta}_{\mathrm{I}}$
λ_j = Lagrange multiplier of the jth active constraint

Superscripts

+ = positive direction
− = negative direction
in = inlet
max = upper limits
min = lower limits
N = nominal values
out = outlet
ss = steady state value
U = upper bounds

Subscripts

i = label of equality constraint
I = label of alterable offline uncertainty parameters
II = label of unalterable uncertainty parameters
j = label of inequality constraint

■ REFERENCES

(1) Grossmann, I. E.; Floudas, C. A. Active Constraint Strategy for Flexibility Analysis in Chemical Process. *Comput. Chem. Eng.* **1987**, *11*, 675–693.

(2) Lima, F. V.; Jia, Z.; Ierapetritou, M.; Georgakis, C. Similarities and Differences between the Concepts of Operability and Flexibility: The Steady-State Case. *AIChE J.* **2010**, *56*, 702–716.

(3) Lima, F. V.; Georgakis, C. Design of Output Constraints for Model-based Non-square Controllers Using Interval Operability. *J. Process Control* **2008**, *18*, 610–620.

(4) Lima, F. V.; Georgakis, C.; Smith, J. F.; Schnelle, P. D.; Vinson, D. R. Operability-Based Determination of Feasible Control Constraints for Several High-Dimensional Nonsquare Industrial Processes. *AIChE J.* **2009**, 1249–1261.

(5) Malcom, A.; Polan, J.; Zhang, L.; Ogunnaike, B. A.; Linninger, A. A. Integrating Systems Design and Control Using Dynamic Flexibility Analysis. *AIChE J.* **2007**, *53*, 2048–2061.

(6) Bansal, V.; Perkins, J. D.; Pistikopoulos, E. N. Flexibility Analysis and Design of Linear Systems by Parametric Programming. *AIChE J.* **2000**, *46*, 335–354.

(7) Bansal, V.; Perkins, J. D.; Pistikopoulos, E. N. Flexibility Analysis and Design Using a Parametric Programming Framework. *AIChE J.* **2002**, *48*, 2851–2867.

(8) Dimitriadis, V. D.; Pistikopoulos, E. N. Flexibility Analysis of Dynamic Systems. *Ind. Eng. Chem. Res.* **1995**, *34*, 4451–4462.

(9) Floudas, C. A.; Gümüş, Z. H.; Ierapetritou, M. G. Global Optimization in Design under Uncertainty: Feasibility Test and Flexibility Index Problems. *Ind. Eng. Chem. Res.* **2001**, *40*, 4267–4282.

(10) Grossmann, I. E.; Halemane, K. P. Decomposition Strategy for Designing Flexible Chemical Plants. *AIChE J.* **1982**, *28*, 686–694.

(11) Halemane, K. P.; Grossmann, I. E. Optimal Process Design under Uncertainty. *AIChE J.* **1983**, *29*, 425–433.

(12) Swaney, R. E.; Grossmann, I. E. An Index for Operational Flexibility in Chemical Process Design. Part I: Formulation and Theory. *AIChE J.* **1985**, *31*, 621–630.

(13) Swaney, R. E.; Grossmann, I. E. An Index for Operational Flexibility in Chemical Process Design. Part II: Computational Algorithms. *AIChE J.* **1985**, *31*, 631–641.

(14) Chang, C. T.; Li, B. H.; Liou, C. W. Development of a Generalized Mixed Integer Nonlinear Programming Model for Assessing and Improving the Operational Flexibility of Water Network Designs. *Ind. Eng. Chem. Res.* **2009**, *48*, 3496–3504.

(15) Riyanto, E.; Chang, C. T. A Heuristic Revamp Strategy to Improve Operational Flexibility of Water Networks Based on Active Constraints. *Chem. Eng. Sci.* **2010**, *65*, 2758–2770.

(16) Zhou, H.; Li, X. X.; Qian, Y.; Chen, Y.; Kraslawski, A. Optimizing the Initial Conditions To Improve the Dynamic Flexibility of Batch Processes. *Ind. Eng. Chem. Res.* **2009**, *48*, 6321–6326.

(17) Holland, J. H. *Adaptation in Natural and Artificial Systems*; University of Michigan Press: Ann Arbor, MI, 1975.

(18) Goldberg, D. E. *Genetic Algorithms in Search Optimization and Machine Learning*; Addison-Wesley: New York, 1989.

(19) Storn, R.; Price, K. Differential Evolution—A Simple and Efficient Heuristic for Global Optimization over Continuous Spaces. *J. Global Optim.* **1997**, *11*, 341–359.

(20) Storn, R. On the Usage of Differential Evolution for Function Optimization. In *Proceedings of the 1996 Biennial Conference of the North American Fuzzy Information Processing Society (NAFIPS)*; Smith, M. H., Lee, M. A., Keller, J., Yen, J. Eds.; IEEE Press: Piscataway, NJ, 1996; pp 519−523.

(21) Eberhart, R. C.; Kennedy, J. A New Optimizer Using Particle Swarm Theory. In *Proceedings of the Sixth International Symposium on Micro Machine and Human Science*; Nagoya Municipal Industrial Research Institute, IEEE Press: Piscataway, NJ, 1995; pp 39−43.

(22) Kennedy, J.; Eberhart, R. C. Particle Swarm Optimization. In *Proceedings of the IEEE International Conference on Neural Networks*; IEEE Press: Piscataway, NJ, 1995; Vol. 4, pp 1942−1948.

(23) Shi, Y.; Eberhart, R. C. A Modified Particle Swarm Optimizer. In *Proceedings of the IEEE International Con. on Evolutionary Computation*; IEEE Press: Piscataway, NJ, 1998; pp 69−73.

(24) Pedersen M. E. H. Tuning & Simplifying Heuristical Optimization. Ph.D. Thesis, School of Engineering Sciences, University of Southampton, UK, 2008.

(25) Biegler, L. T.; Grossmann, I. E.; Westerberg, A. W. *Systematic Methods of Chemical Process Design*; Prentice Hall: Englewood Cliffs, NJ, 1997; pp 690−714.

(26) Ferris, M. C. *MATLAB and GAMS: Interfacing Optimization and Visualization Software*; Computer Sciences Department, University of Wisconsin-Madison: Madison, WI, 2005; available at http://www.cs.wisc.edu/math-prog/matlab.html (Accessed May 2011).

(27) Riyanto, E. A Heuristical Revamp Strategy to Improve Operational Flexibility of Existing Water Networks. M.S. Thesis, National Cheng Kung University, Tainan, Taiwan, 2009.

(28) Liu, J.; Lampinen, J. On Setting the Control Parameter of the Differential Evolution Method. In *Proceedings of the 8th International MENDEL Conference on Soft Computing*; Brno University of Technology: Brno, Czech Republic, 2002; pp 11−18, ISBN 80-214-2135-5.

(29) Zaharie, D. Critical Values for the Control Parameters of Differential Evolution Algorithms. In *Proceedings of the 8th International MENDEL Conference on Soft Computing*; Brno University of Technology: Brno, Czech Republic, 2002; pp 62−67, ISBN 80-214-2135-5.