Computers and Chemical Engineering 57 (2013) 151–158

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

A mathematical programming formulation for temporal flexibility analysis

Vincentius Surya Kurnia Adi, Chuei-Tin Chang*

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

ARTICLE INFO

Article history:
Received 14 September 2012
Received in revised form 29 March 2013
Accepted 1 April 2013
Available online 6 April 2013

Keywords:
Dynamic flexibility
Temporal flexibility
Process design
Differential quadrature

ABSTRACT

Realistic chemical processes are often operated in the presence of complex and uncertain dynamics. While an ill designed system may become inoperable due to variations in some process parameters at certain instances, the cumulative effects of temporary disturbances in finite time intervals can also result in serious consequences. The latter issue is studied in the present study on the basis of a novel concept – *temporal flexibility*. Specifically, the mathematical program used for evaluating the corresponding performance measure is built with a dynamic system model, which usually consists of a set of differential-algebraic equations (DAEs). The numerical technique of differential quadrature (DQ) is adopted to approximate these DAEs with equality constraints. As a result, any solution strategy for the conventional steady-state flexibility analysis is applicable. Two examples, a simple liquid storage tank and a solar thermal driven membrane distillation desalination process, are adopted to demonstrate the usefulness of temporal flexibility analysis. All results obtained in case studies show that the proposed approach is convenient and effective for assessing realistic issues in operating complex dynamic chemical processes.

1. Introduction

Dealing with uncertainties is one of the practical issues in designing and operating chemical plants. These so-called uncertainties may arise either from random exogenous disturbances (such as those in feed qualities, product demands, and environmental conditions, etc.) or from uncharacterizable variations in the internal parameters (such as heat transfer coefficients, reaction rate constants, and other physical properties) (Lima & Georgakis, 2008; Lima, Georgakis, Smith, Schnelle, & Vinson, 2009; Lima, Jia, Ierapetritou, & Georgakis, 2010; Malcom, Polan, Zhang, Ogunnaike, & Linninger, 2007). The ability of a chemical process to maintain feasible operation despite uncertain deviations from the nominal states is often referred to as its *operational flexibility* (Swaney & Grossmann, 1985a, 1985b), which is clearly a feature of key importance that must be incorporated into the design considerations. This requirement can only be satisfied if a quantitative performance measure can be made available. To this end, various approaches to facilitate flexibility analysis have been proposed in numerous studies published in the literature (Adi & Chang, 2011; Bansal, Perkins, & Pistikopoulos, 2000, 2002; Floudas, Gunus, & Ierapetritou, 2001; Grossmann & Floudas, 1987; Grossmann & Halemane, 1982; Halemane & Grossmann, 1983; Lima & Georgakis, 2008; Lima et al., 2009, 2010; Malcom et al., 2007; Ostrovski, Achenie, Wang, & Volin, 2001; Ostrovski & Volin, 2002; Swaney & Grossmann, 1985a, 1985b; Varvarezos, Grossmann, & Biegler, 1995; Volin & Ostrovski, 2002).

The *flexibility index* (FI) was first defined by Swaney and Grossmann (1985a, 1985b) for use as an unambiguous gauge of the feasible region in the parameter space. Specifically, this FI is associated with the maximum allowable deviations of the uncertain parameters from their nominal values, by which feasible operation can be assured with proper manipulation of the control variables. Swaney and Grossmann (1985b) also showed that, under certain convexity assumptions, critical points that limit feasibility and/or flexibility must lie on the vertices of the uncertain parameter space. Grossmann and Floudas (1987) later exploited the fact that sets of active constraints are responsible for limiting the flexibility of a design and developed a mixed integer nonlinear programming (MINLP) model accordingly. Similar flexibility analysis has also been carried out in a series of subsequent studies to produce resilient grassroots and revamp designs (Chang, Li, & Liou, 2009; Riyanto & Chang, 2010). Since the steady-state material-and-energy balances are used as the equality constraints in the aforementioned MINLP model (Grossmann & Floudas, 1987; Ostrovski et al., 2001; Ostrovski & Volin, 2002; Swaney & Grossmann, 1985a, 1985b; Varvarezos et al., 1995; Volin & Ostrovski, 2002), FI can be viewed as a performance indicator of the *continuous* process under consideration (Pistikopoulos & Grossmann, 1988a, 1988b, 1989a, 1989b; Petracci, Hoch, & Cliche, 1996). On the other hand, several alternative approaches

* Corresponding author. Tel.: +886 6 275 7575x62663; fax: +886 6 234 4496.
E-mail addresses: ctchang@mail.ncku.edu.tw, chueitinchang@msn.com (C.-T. Chang).

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http://dx.doi.org/10.1016/j.compchemeng.2013.04.001

Nomenclature

Acronyms

AGMD	air-gap membrane distillation
DAE	differential-algebraic equation
DQ	differential quadrature
FI	flexibility index
HDMR	high dimensional model representation
KKT	Karush–Kuhn–Tucker
MINLP	mixed integer nonlinear programming
SF	stochastic flexibility
SMDDS	solar-driven membrane distillation desalination system

Variables

a	time range start
b	time range end
d	vector of design variables
g	inequality constraints
h	equality constraints, height
k	constant
m	mass flow rate
r	flow rate ratio
t	time
x	vector of state variables
z	vector of control variables
A	cross-sectional area
H	operation horizon
M	total volumetric mass
Cp	heat capacity
FI	flexibility index
I	set of equality constraints
J	set of inequality constraints

Greek letters

δ	deviation due to uncertainties
Δ	expected deviations
π	phi constant
ρ	liquid density
τ	time
θ	uncertain parameters
$\boldsymbol{\theta}$	vector of uncertain parameters
Θ	acumulated uncertainty parameters

Superscripts

+	positive direction
−	negative direction
N	nominal values
0	variable at $t=0$
L	liquid state

Subscripts

d	dynamic
f	fluid
i	label of equality constraint, weighting coefficient, location of zeros
j	label of inequality constraint, weighting coefficient, location of zeros
k	label of state variables
r	Chebyshev roots
s	steady-state
in	inlet
out	outlet
N	number of Chebyshev roots
mem	membrane
CL	cold liquid
DT	distillate tank
HL	hot liquid
HX	heat exchanger
MD	membrane distillation
SA	solar absorber
ST	storage tank
STL	solar thermal loop

have also been proposed to address the uncertainty issues from a stochastic viewpoint (Pistikopoulos & Mazzuchi, 1990; Pistikopoulos, Mazzuchi, & Van Rijn, 1990; Straub & Grossmann, 1990, 1992, 1993). Pistikopoulos et al. (1990) developed the combined flexibility-availability index, while Straub and Grossmann (1990) incorporated the stochastic uncertainty into flexibility analysis model. Finally, notice that Banerjee and Ierapetritou (2002, 2003) addressed the feasibility issues for processes where the closed-form models are not available. The feasibility analysis was facilitated with input-output *high dimensional model representation* (HDMR) mapping (Banerjee, Pal, & Maiti, 2010; Sahinidis, 2004). The feasible region was treated by Banerjee and Ierapetritou (2005) as an object, and the shape reconstruction techniques were used to approximate the feasible parameter space. The key to using this black-box method for performing feasibility analysis lies in balancing the need to minimize expensive and time consuming sampling with the necessity of accurately mapping the feasible region and strictly avoiding overprediction. Boukouvala and Ierapetritou (2012) recently utilized the Kriging interpolating technique to determine the effect(s) of parameter uncertainty on the basis of only a set of input uncertainties. It is clear from the above discussions that more than one type of models may be available for steady-state flexibility/feasibility analysis. In the present study, the original deterministic approach is still adopted to strike a proper compromise between model fidelity and simplicity.

As indicated by Dimitriadis and Pistikopoulos (1995), the operational flexibility of a *dynamic* system should be evaluated differently. By adopting a system of differential algebraic equations (DAEs) as the model constraints, these authors developed a mathematical programming formulation for dynamic flexibility analysis. Clearly this practice is more rigorous than that based on the steady-state model since, even for a continuous process, the operational flexibility cannot be adequately characterized without accounting for the control dynamics. In an earlier study, Brengel and Seider (1992) advocated the need for design and control integration. The integration of flexibility and controllability in design was discussed extensively by several other groups (Aziz & Mujtaba, 2002; Bahri, Bandoni, & Romagnoli, 1997; Bansal, Perkins, & Pistikopoulos, 1998; Chacon-Mondragon & Himmelblau, 1996; Georgiadis & Pistikopoulos, 1999; Malcom et al., 2007; Mohideen, Perkins, & Pistikopoulos, 1996). Soroush and Kravaris (1993a, 1993b) addressed the issues concerning flexible operation for batch reactors. The effects of uncertainty on the dynamic behavior of chemical processes were also studied by Walsh and Perkins (1994), with particular reference to the wastewater neutralization processes. White, Perkins, and Espie (1996) presented an approach for the evaluation of the switchability of a proposed design, i.e., its ability to perform satisfactorily when moving between different operating points. Dimitriadis, Shah, and Pantelides (1997) studied the feasibility problem from the safety verification point of view. Zhou, Li, Qian, Chen, and Kraslawski (2009) utilized a similar approach to assess the operational flexibility of batch systems. This problem is considered to be more challenging since the nature of inherent system dynamics is dependent upon the initial conditions.

Notice that, in all aforementioned dynamic flexibility analyses, the nominal values of uncertain parameters and the anticipated positive and negative deviations in these parameters are assumed to be available at every instance over the entire time horizon of operation life. The corresponding flexibility index can be uniquely determined on the basis of dynamic system model and also such *a priori* information. However, while an ill designed system may become inoperable due to variations in some process parameters at certain instances, the cumulative effects of temporary disturbances in finite time intervals can also result in serious consequences. The latter scenario is usually ignored in the traditional dynamic flexibility analysis, but it is in fact a more probable event in practical applications. To address this issue, a new mathematical programming model is developed in this work for computing the corresponding performance measure, which will later be referred to as the *temporal flexibility index*. Realistic process improvements can then be introduced on the basis of this novel approach in flexibility analysis.

The rest of the paper is organized as follows. The conventional formulation is first reviewed in the next section, which includes the MINLP models for stead-state and dynamic flexibility analyses. The development of a new model for computing the temporal flexibility index is then presented in Section 3. The DAEs embedded in this model can be transformed into algebraic equations by approximating the derivatives with differential quadratures (DQs) at the selected nodes on time horizon. This model discretization procedure is described in Section 4. In the above two sections, a simple liquid storage example is also given to provide clear illustration of the proposed formulation and the required solution steps. An additional more realistic example, i.e., the solar driven membrane distillation desalination system (SMDDS), is presented in Section 5 to demonstrate the applicability and usefulness of the proposed model. Finally, conclusions are drawn in Section 6.

2. Conventional formulations for flexibility analysis

To facilitate clear explanation of the proposed concept, let us briefly consider the conventional formulations for flexibility analysis. As mentioned previously, the algebraic constraints are adopted in the original models (Swaney & Grossmann, 1985a, 1985b). For illustration convenience, the following label sets should be first defined:

$$I = \{i | i \text{ is the label of an equality constraint}\} \quad (1)$$

$$J = \{j | j \text{ is the label of an inequality constraint}\} \quad (2)$$

The general design model can thus be expressed accordingly as

$$f_i(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) = 0, \quad \forall i \in I \quad (3)$$

$$g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0, \quad \forall j \in J \quad (4)$$

where, f_i is the ith equality constraint in the design model (e.g., the mass or energy 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; $\boldsymbol{\theta}$ denotes the vector of uncertain parameters. Given a nominal parameter value $\boldsymbol{\theta}^N$ and the corresponding expected deviations in the positive and negative directions ($\Delta\boldsymbol{\theta}^+$ and $\Delta\boldsymbol{\theta}^-$), the uncertain parameters can be constrained as

$$\boldsymbol{\theta}^N - \delta\Delta\boldsymbol{\theta}^- \leq \boldsymbol{\theta} \leq \boldsymbol{\theta}^N + \delta\Delta\boldsymbol{\theta}^+ \quad (5)$$

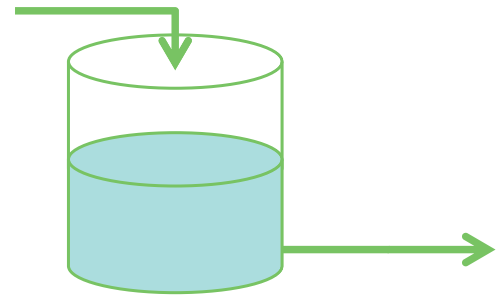

Fig. 1. A liquid buffer tank.

where δ is a positive scalar variable to be determined with the flexibility index model.

In the original formulation, the flexibility index represents the largest deviation that the design can accommodate while remaining feasible, i.e., satisfying Eqs. (3) and (4). This steady-state flexibility index can be determined by solving the following model:

$$\mathrm{FI_s} = \max \quad \delta \quad (6)$$

subject to the constraints in Eqs. (3) and (5) and those given below:

$$\max_{\theta} \ \min_{z} \ \max_{j} \ g_j(\mathbf{d}, \mathbf{z}, \mathbf{x}, \boldsymbol{\theta}) \leq 0 \quad (7)$$

It should be noted that $\mathrm{FI_s} \geq 1$ indicates that the flexibility target is reached for the corresponding steady-state operations.

As mentioned previously, Dimitriadis and Pistikopoulos (1995) suggested replace the equality constraints in Eq. (3) with a system of differential-algebraic equations, i.e.

$$f_i(\mathbf{d}, \mathbf{z}(t), \mathbf{x}(t), \dot{\mathbf{x}}(t), \boldsymbol{\theta}(t)) = 0 \quad (8)$$

where, $t \in [0, H], \quad i \in I$, and $\mathbf{x}(0) = \mathbf{x}^0$. Thus, the dynamic flexibility index can be computed with the following model:

$$\mathrm{FI_d} = \max \quad \delta \quad (9)$$

subject to Eq. (8) and

$$\max_{\boldsymbol{\theta}(t)} \ \min_{\mathbf{z}(t)} \ \max_{j,t} \ g_j(\mathbf{d}, \mathbf{z}(t), \mathbf{x}(t), \boldsymbol{\theta}(t), t) \leq 0 \quad (10)$$

$$\boldsymbol{\theta}^N(t) - \delta\Delta\boldsymbol{\theta}^-(t) \leq \boldsymbol{\theta}(t) \leq \boldsymbol{\theta}^N(t) + \delta\Delta\boldsymbol{\theta}^+(t) \quad (11)$$

Note that time is introduced in this model as an independent variable since it is necessary to characterize the system dynamics. Notice also that the scope of dynamic flexibility index obviously covers the *entire* operation horizon [0,*H*]. However, there is also a need to determine a "short-term" flexibility index in practice for the purpose of assessing the effectiveness of emergency plans. It is important to note that the cumulative effects of temporary disturbances cannot be properly assessed with the aforementioned formulations. A simple scenario can be used to clarify this point:

Let us consider the buffer tank in Fig. 1. The dynamic model of this system can be written as

$$A\frac{dh}{dt} = \theta(t) - k\sqrt{h} \quad (12)$$

where, h denotes the height of liquid level (m); θ denotes the feed flow rate ($m^3\,min^{-1}$); A (=5 m^2) is the cross-sectional area of the tank; k $(=\sqrt{5}/10 \ \ m^{5/2} \ \ min^{-1})$ is a proportional constant. For illustration purpose, the following assumptions are adopted:

- The height of tank is 10 m;
- The system is normally operated at steady state and thus the time horizon is semi-infinite, i.e., $0 \le t < \infty$.
- The feed flow rate is the only uncertain parameter in this example and its nominal value at steady state is $\boldsymbol{\theta}^N(t) = 0.5\ \ \text{m}^3\ \ \text{min}^{-1}$. Therefore, the nominal height of liquid level can be determined to be 5 m.

If the upstream feed supply may be interrupted for at most 125 min during operation, it is obviously desirable to find out if the capacity of this buffer tank is enough for maintaining a prescribed minimum flow (or minimum height) at all time. However, this question cannot be answered by performing the conventional dynamic flexibility analysis since the uncertain parameter(s) in Eq. (11) is constrained at every time instance without considering the cumulative effects.

3. Temporal flexibility index

Let us assume that the variations in uncertain parameters are possible only within a finite time interval $[t_0, t_1] \subset [0, H]$. To characterize the cumulative effects, let us integrate equation (11), i.e.

$$-\delta \int_{t_0}^{t_1} \Delta\boldsymbol{\theta}(\tau)^- d\tau \le \int_{t_0}^{t_1} (\boldsymbol{\theta}(\tau) - \boldsymbol{\theta}(\tau)^N) d\tau \le \delta \int_{t_0}^{t_1} \Delta\boldsymbol{\theta}(\tau)^+ d\tau \qquad (13)$$

Since the expected maximum deviations in uncertain parameters should be regarded as given information, the expected *net* positive and negative cumulated deviations over interval $[t_0, t_1]$ can also be computed in advance. Let us introduce the following definitions to simplify notation:

$$\Delta\Theta^- = \int_{t_0}^{t_1} \Delta\boldsymbol{\theta}(\tau)^- d\tau \qquad \Delta\Theta^+ = \int_{t_0}^{t_1} \Delta\boldsymbol{\theta}(\tau)^+ d\tau \qquad (14)$$

and

$$\Theta(t) = \int_{t_0}^{t} (\boldsymbol{\theta}(\tau) - \boldsymbol{\theta}(\tau)^N) d\tau \qquad (15)$$

In this study, a stricter constraint is imposed upon the aforementioned accumulated effects so as to ensure operational safety. Specifically, Eq. (13) is modified as follows

$$-\delta\Delta\Theta^- \le \Theta(t) \le \delta\Delta\Theta^+ \qquad (16)$$

Furthermore, since the time interval $[t_0, t_1]$ itself may be uncertain, Eq. (15) can be rewritten as:

$$\frac{d}{dt}\Theta(t) = \boldsymbol{\theta}(t) - \boldsymbol{\theta}^N(t) \qquad (17)$$

where $\Theta(0) = \mathbf{0}$ and $t \in [0, H]$. Eqs. (8), (10), (11), (16) and (17) can then be used as the constraints of a mathematical programming model to determine the temporal flexibility index FI_t by maximizing the scalar variable δ.

To illustrate the above idea, let us again consider the simple buffer tank presented in Fig. 1. Based on the aforementioned assumption that the upstream feed supply may be interrupted for at most 125 min, one can determine the maximum values of the accumulated negative and positive deviations according to Eq. (14), i.e.

$$\Delta\Theta^- = (0.5 - 0) \times 125 = 62.5\ \ \text{m}^3 \qquad \Delta\Theta^+ = 0\ \ \text{m}^3 \qquad (18)$$

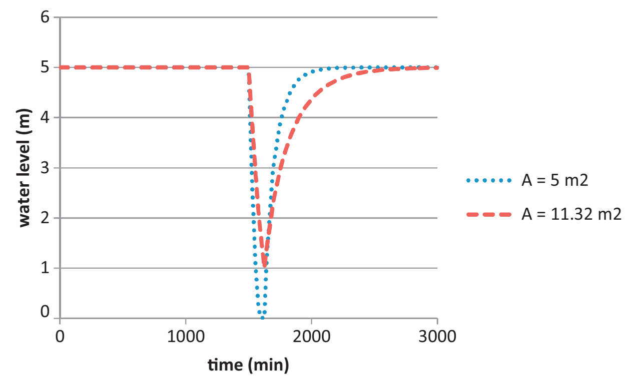

Fig. 2. Responses to the anticipated disturbance profile, i.e., the upstream feed supply is interrupted for 125 min.

Let us assume that, due to the operational requirement of downstream unit(s), the outlet flow rate of buffer tank must be kept above $\sqrt{5}/10\ \ \text{m}^3\ \ \text{min}^{-1}$. Thus, the minimum allowable height of its liquid level should be 1 m. For a tank of cross-sectional area $A = 5\ \text{m}^2$, the resulting temporal flexibility index can be determined to be 0.643. In other words, such a buffer system is not flexible enough to withstand the anticipated feed outage. It can also be found that FI_t can be raised to 1 if the cross-sectional area is increased to 11.32 m^2.

The above predictions can be verified in numerical simulation studies. The simulation results of anticipated scenarios are presented in Fig. 2. In both cases, the feed was cut off at 1500 min and resumed at 1625 min. It can be observed that

1. the smaller tank ($A = 5\ \ \text{m}^2$) is quickly emptied after 100 min (at 1600 min), and
2. the liquid level in the bigger tank ($A = 11.32\ \ \text{m}^2$) is always above 1 m.

Notice also that, if the maximum anticipated values in Eq. (18) are adopted in the proposed flexibility analysis, the inequality constraints in Eq. (16) can be satisfied by infinitely many disturbance profiles. The predictions of temporal flexibility analysis should be valid in all such scenarios. For example, for the two buffer tanks mentioned above, let us consider the outcomes of another disturbance, i.e., a temporary reduction of feed supply rate to 0.1875 m^3 min^{-1} for 200 min. The most negative value of the accumulated deviation in these two scenarios should be

$$\min_t \ \Theta(t) = (0.1875 - 0.5) \times 200 = -62.5\ \ \text{m}^3 \qquad (19)$$

From the corresponding simulation results presented in Fig. 3, it can be seen that almost the same trends can be identified. In

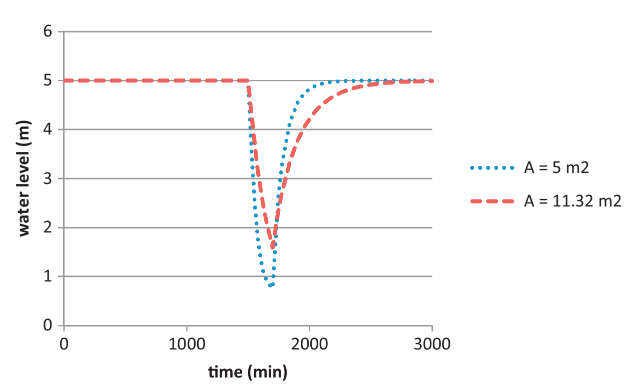

Fig. 3. Responses to the disturbance profile that satisfies Eq. (19), i.e., a temporary reduction of feed supply rate to 0.1875 m^3 min^{-1} for 200 min.

fact this observation can also be made for other deviation profiles as long as Eq. (19) holds. Finally, it should be noted that the liquid height should always stay above 1 m if the temporarily reduced feed supply rate is higher than $\sqrt{5}/10\ \ \mathrm{m}^3\ \ \mathrm{min}^{-1}$. Therefore, the theoretical implications of temporal flexibility index can be summarized as follows:

If $FI_t < 1$, then the given buffer system cannot withstand at least some of the temporary disturbances (in feed supply) that satisfy Eq. (16). If otherwise, then the buffer operation should always be successful.

4. Model discretization with differential quadrature

A simple solution strategy is adopted in the present study for computing the temporal flexibility index. In particular, the DAEs in Eq. (8) are first converted to a system of algebraic equations according to a credible numerical discretization technique and the resulting optimization problem is then solved with any existing algorithm for the steady-state flexibility analysis, e.g., see Biegler et al. (1997).

An effective tool for realizing this strategy is the differential quadrature (DQ) (Bellman & Casti, 1971; Bellman et al., 1972). It should be noted that the accuracy of DQ approximation has been well documented in the literature (e.g., Civan & Sliepcevich, 1984; Quan & Chang, 1989a, 1989b; Chang et al., 1993). The implementation procedure is also very straightforward. Specifically, the derivative of every variable in Eqs. (8) and (17) is approximated with a DQ, i.e., the derivative value at every node is computed according to a weighted sum of the variable values at all nodes in a time element. Let us consider the derivative of state variable x_k (k=1, 2, ...) as an example:

$$\left.\frac{dx_k(t)}{dt}\right|_{t=t_i} = \sum_{j=1}^{N} w_{ij} x_k(t_j), \quad i = 1, 2, \ldots, N \tag{20}$$

Note that the weighting coefficients w_{ij} are dependent only upon the node spacing. Thus, it can be easily deduced from this equation that, by using DQ, any differential equation can be converted to a set of algebraic equations.

Quan and Chang (1989a) further suggested that, in most cases, it is beneficial to use the shifted zeros of a standard Chebyshev polynomial as the selected nodes. This node spacing in an arbitrary interval $t \in [a, b]$ yields the following formulas for calculating the weighting coefficients, i.e.

$$w_{ij} = \frac{r_N - r_1}{b - a} \frac{(-1)^{(i-j)}}{(r_i - r_j)} \sqrt{\frac{(1 - r_j^2)}{(1 - r_i^2)}}, \quad i \neq j \tag{21}$$

$$w_{ii} = \frac{1}{2} \frac{r_N - r_1}{b - a} \frac{r_i}{(1 - r_i^2)} \tag{22}$$

where $i, j = 1, 2, \ldots, N$ and the locations of Chebyshev zeros in the standard interval [−1,+1] are

$$r_i = \cos\frac{(2i - 1)\pi}{2N} \tag{23}$$

As an example, Eq. (12) can be transformed into the following set of algebraic equations:

$$A \sum_{j=1}^{N} w_{ij} h(t_j) = \theta(t_i) - k\sqrt{h(t_i)}, \quad i = 1, 2, \ldots, N \tag{24}$$

where w_{ij} is the weighting coefficients for the 1st order derivatives. For the motivational example presented in the previous sections, a total of 300 evenly distributed elements were selected over a simulation horizon [0,3000]. In each time element, five nodes were placed ($N = 5$) at the Chebyshev roots. The corresponding weighting coefficients can be determined according to Eqs. (21)–(23) and they are listed in Table 1.

Table 1
Weighting coefficients for $b - a = 10$ and $N = 5$.

j	i = 1	2	3	4	5
1	0.900853662	−0.2	0.061803	−0.04721	0.1
2	1.370820393	0.050203	−0.2618	0.161803	−0.32361
3	−0.647213595	0.4	3.57E−34	−0.4	0.647214
4	0.323606798	−0.1618	0.261803	0.050203	−1.37082
5	−0.1	0.047214	−0.0618	0.2	0.900854

Thus, the time profiles of state and control variables can be constructed in each time element with the Chebyshev polynomials. Continuity of every profile at the border point of each pair of adjacent elements can be enforced with a boundary condition, and the element length and number can be adjusted to achieve satisfactory accuracy.

5. Application example – SMDDS

A large-scale solar thermal driven membrane distillation desalination system (SMDDS) is adopted in this paper to demonstrate the usefulness of temporal flexibility analysis in practical applications. The flow diagram of SMDDS is depicted in Fig. 4. The major components in this system are: (1) the solar absorber, (2) the heat storage tank, (3) the counter-flow shell-and-tube heat exchanger, (4) the air-gap membrane distillation (AGMD) modules, and (5) the distillate tank. The thermal storage circulation fluid, after taking in thermal energy via the solar absorber, is split into two streams. Both streams eventually enter the heat exchanger. One of them is first fed into the thermal storage tank, while the other bypasses it. A step controller is used to maintain the flow ratio of $m_{f,ST}/m_{f,STL}$ (i.e., $r_{f,ST}$) at 0.3 when the output temperature of solar absorber is above 45 °C in daytime operation. When there is no solar irradiation, the system is switched to the night-time operation mode.

The solar irradiation rate $I(t)$ is regarded as an uncertain parameter in this example. Its nominal profile, i.e., $I^N(t)$, can be found in Fig. 5 and the expected deviations are set at ±10% of the nominal levels. The water demand rate $m_{f,DTout}(t)$ is treated as another uncertain parameter. Its nominal value is assumed to be constant at 25 m^3/h (416.667 kg/min), which is sufficient to support 1% of the municipal population (about 2000 people) in East District of Tainan City, Taiwan (Taiwanese Government Consuming Water Statistics Database Annual Reports, 2010). The expected positive deviation in

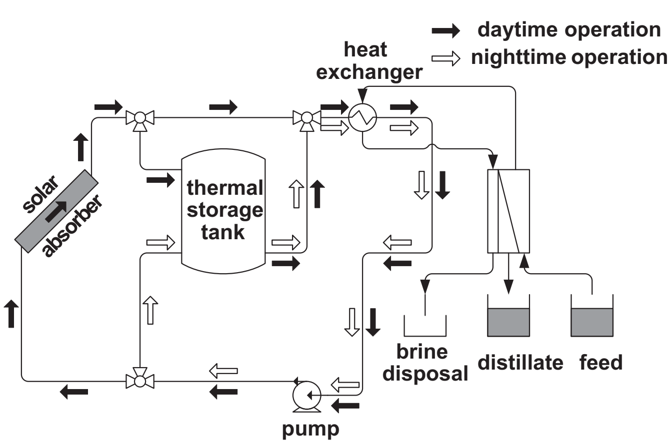

Fig. 4. SMDDS process.

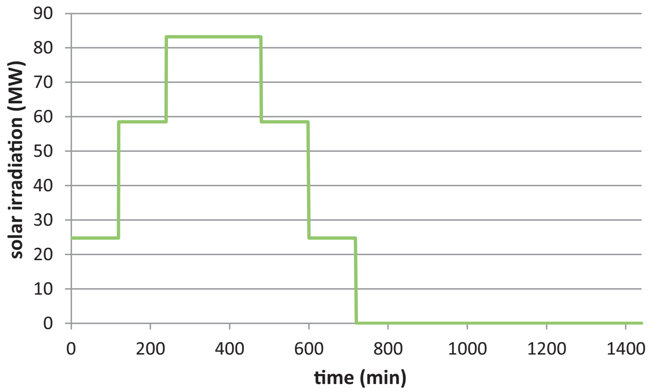

Fig. 5. Nominal solar irradiation profile.

$m_{f,\mathrm{DTout}}$ is 10% of its nominal value (which starts at t = 240 min and lasts for 120 min), while the negative counterpart is a 5% decrease from the nominal level within time interval [240, 360] min.

Let us assume that, in the beginning of every operation cycle, the entire system is at the same temperature, i.e., 25 °C. A constant circulation rate of 500 m^3/h is supposed to be maintained in the solar thermal loop ($m_{f,\mathrm{STL}}$), while the nominal flow rate in the membrane distillation loop ($m_{f,\mathrm{MD}}$) is 200 m^3/h. It is assumed that the latter flow rate can be manipulated within ±20% of its nominal value in order to compensate the effects of uncertain disturbances. The cold sea water is first heated in the AGMD module via energy exchange with the hot fluid, then further heated in the heat exchanger and finally returned to the hot side of the module as the hot fluid feed. The condensed permeate (distillate), i.e., the water transported through the membrane, is collected in the distillate tank and then directly distributed to domestic users. The equipment specifications of the SMDDS in this study are listed in Table 2 (Chang et al., 2012).

Following is a brief description of the mathematical model used in the present example:

- Solar absorber

  Thermal energy is transported to the circulation fluid in solar absorber. The dynamic energy balance equation for the fluid can be written as:

$$\frac{dT_{f,\mathrm{SAout}}}{dt} = -L_{\mathrm{SA}}\frac{m_{f,\mathrm{SA}}}{M_{f,\mathrm{SA}}}\frac{T_{f,\mathrm{SAout}} - T_{f,\mathrm{SAin}}}{L_{\mathrm{SA}}} + \frac{A_{\mathrm{SA}}I(t)}{M_{f,\mathrm{SA}}Cp_f^L} \tag{25}$$

Table 2
Equipment specifications.

Solar absorber module (2000 units)	
Mass, $M_{f,\mathrm{SA}}$	900 kg
Absorber area, A_{SA}	45 m^2
Length, L_{SA}	5 m
Heat capacity, Cp_f^L	4.2 kJ/kg K
Liquid density, ρ	1000 kg/m^3
Thermal storage tank (1 unit)	
Total initial mass of water, $M_{f,\mathrm{ST}}$	200,000 kg
Height of tank, H_{ST}	8 m
AGMD module (2000 units)	
Membrane area, A_{mem}	40 m^2
Membrane constant, K_{mem}	4.7 × 10^{-11} kg/m^2 K
Distillate tank (1 unit)	
Total initial mass of water, $M_{f,\mathrm{DT}}$	250,000 kg
Height of tank, H_{DT}	10 m

$$m_{f,\mathrm{SA}} = \begin{cases} m_{f,\mathrm{STL}} & \text{if} \quad I(t) > 0 \\ 0 & \text{otherwise} \end{cases} \tag{26}$$

$$T_{f,\mathrm{SAout}} \le 100 \quad {}^\circ\mathrm{C} \tag{27}$$

$$m_{f,\mathrm{STL}} = (1 - r_{f,\mathrm{ST}})m_{f,\mathrm{SA}} + m_{f,\mathrm{ST}} \tag{28}$$

All symbols used in the above formulation are defined in the Nomenclature section. For the sake of brevity, these definitions are omitted here. Notice also that, in Eq. (27), the outlet temperature is required to be below 100 °C so as to avoid evaporation. Finally, heat loss is neglected because the absorber is assumed to be well insulated.

- Thermal storage tank

  By assuming that the fluid inside the thermal storage tank well mixed, the corresponding energy balance equation can be expressed as

$$M_{f,\mathrm{ST}}\frac{dT_{f,\mathrm{STout}}}{dt} = r_{f,\mathrm{ST}}m_{f,\mathrm{STL}}(T_{f,\mathrm{STin}} - T_{f,\mathrm{STout}}) \tag{29}$$

$$r_{f,\mathrm{ST}} = \begin{cases} 0.3 & \text{if} \quad T_{f,\mathrm{SAout}} \ge 45 \quad {}^\circ\mathrm{C} \\ 0 & \text{otherwise} \end{cases} \tag{30}$$

- Heat exchanger

  The hot fluid used in the counter-flow heat exchanger comes from the thermal storage tank and/or solar absorber, while the cold fluid is the sea water from the membrane distillation module. The dynamics in this unit are ignored and a steady-state energy balance is used to model the heat-exchange process

$$m_{f,\mathrm{MD}}(T_{f,\mathrm{HX,HLout}} - T_{f,\mathrm{MD,CLout}}) = (1 - r_{f,\mathrm{ST}})m_{f,\mathrm{SA}}(T_{f,\mathrm{SAout}} - T_{f,\mathrm{SAin}}) + m_{f,\mathrm{ST}}(T_{f,\mathrm{STout}} - T_{f,\mathrm{STin}}) \tag{31}$$

- AGMD module

  A simplified model is developed for the AGMD module. It is assumed that the mass flux is a function of the total heat put into the module. Specifically, the membrane mass flux can be expressed as

$$N_{\mathrm{mem}} = k_{\mathrm{mem}}A_{\mathrm{mem}}m_{f,\mathrm{MD}}(T_{f,\mathrm{HX,HLout}} - T_{f,\mathrm{MD,CLout}}) \tag{32}$$

$$0.8m_{f,\mathrm{MD}}^N \le m_{f,\mathrm{MD}} \le 1.2m_{f,\mathrm{MD}}^N \tag{33}$$

$$T_{f,\mathrm{HX,HLout}} \le 90 \quad {}^\circ\mathrm{C} \tag{34}$$

where $m_{f,\mathrm{MD}}^N = 200 \quad \mathrm{m}^3/\mathrm{h}$. Note that the mass flow rate in membrane distillation loop ($m_{f,\mathrm{MD}}$) is treated as a control variable which is allowed to vary ±20% from its nominal value. Note also that the hot fluid temperature in the module is not allowed to exceed 90 °C to avoid membrane damage.

- Distillate tank

  The cross section area of the distillate tank is assumed to be 50 m^2. The maximum water level allowed is 10 m while the initial water level is at 5 m. The corresponding model can be written as

$$m_{f,\mathrm{DTin}} = N_{\mathrm{mem}} \tag{35}$$

$$\rho A_{\mathrm{DT}}\frac{dh_{\mathrm{DT}}}{dt} = m_{f,\mathrm{DTin}} - m_{f,\mathrm{DTout}} \tag{36}$$

$$0 \le h_{\mathrm{DT}} \le 10 \quad \mathrm{m} \tag{37}$$

- Periodic operation constraints

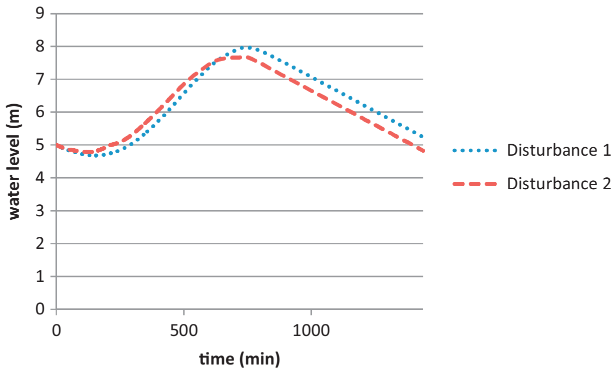

Fig. 6. Water level in distillate tank (h_{DT}) at 100% disturbance loads (disturbance 1: +10% solar irradiation, −5% water demand, $t \in [120, 480]$ min, −20% $m_{f,MD}$; disturbance 2: −10% solar irradiation, +10% water demand, $t \in [240, 360]$ min, +20% $m_{f,MD}$).

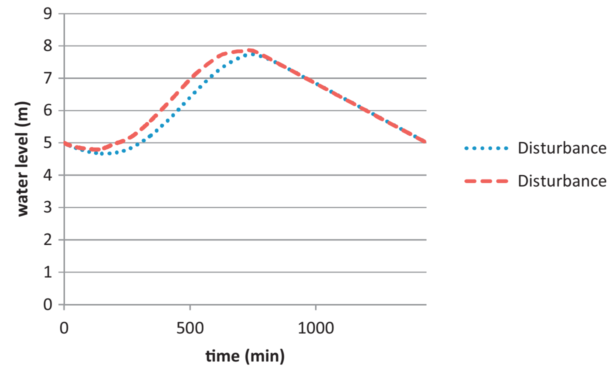

Fig. 7. Water level in distillate tank (h_{DT}) at 70.636% disturbance loads (disturbance 1: +7.636% solar irradiation, −3.5318% water demand, $t \in [120, 480]$ min, −20% $m_{f,MD}$; disturbance 2: −7.636% solar irradiation, +7.636% water demand, $t \in [240, 360]$ min, +20% $m_{f,MD}$).

To maintain cyclic operation, the following equality and inequality constraints are imposed upon the initial and final values of state variables:

$$T_{f,\text{SAout}}(0) = T_{f,\text{SAout}}(H)$$
$$T_{f,\text{STout}}(0) = T_{f,\text{STout}}(H) \qquad (38)$$
$$T_{f,\text{HX,HLout}}(0) = T_{f,\text{HX,HLout}}(H)$$

$$h_{DT}(0) \leq h_{DT}(H) \qquad (39)$$

On the basis of the aforementioned constraints, a mathematical model can be constructed to compute the temporal flexibility index. To solve this optimization problem, the time horizon (24 h) is divided into 360 time elements, while the number of Chebysev nodes in each element is set to be five (5). The temporal flexibility in this case was found to be 0.70636. Since FI_t is less than one, one can conclude that the system cannot overcome some of the anticipated disturbances. The corresponding profile of water level in the distillate tank is given in Fig. 6. Note that Eq. (39) is violated because the disturbances are too large to be compensated with the control variable $m_{f,MD}$.

Intuitively, two simple revamp strategies can be adopted to achieve the desired target of $\text{FI}_t = 1$ without replacing the solar absorber and/or AGMD module, i.e.

1. relaxing the upper and lower limits of the control variable, and
2. reducing the demand loads.

The former can be realized by raising the pump capacity, while the latter by lowering the total water demand. By following a trial-and-error procedure, it was found that the target of $\text{FI}_t = 1$ can be reached

1. if the upper and lower limits of the control variable are increased to ±32% of the nominal value, or
2. if the anticipated demand loads are at 70.636% of the original levels.

This prediction can be verified with the simulation results presented in Fig. 7.

On the other hand, additional revamp strategies can also be identified by relaxing the active constraints when $\text{FI}_t < 1$. As mentioned previously, this constraint is associated with Eq. (39) and can be attributed to slow water production. Thus, the operational flexibility of SMDDS system can be obviously enhanced by enlarging AGMD size if there is enough budget. Specifically, if A_{mem} is increased to 60% larger than the original area, then the temporary flexibility index FI_t can be raised to 1 without altering control range or demand loads.

6. Conclusions

A novel concept of *temporal flexibility* is proposed in this study to address the practical issues caused by short-term disturbances that may occur in operating the chemical plants. A generic mathematical programming model is formulated accordingly for characterizing the corresponding performance measure. This formulation can be transformed into the conventional steady-state flexibility index model by approximating every embedded derivative with a differential quadrature (DQ) and, thus, all existing solution strategies are applicable. Two examples are reported in this paper to demonstrate the feasibility and usefulness of the proposed approach. Although satisfactory results have been obtained, there are still a couple of unsettled issues left for future studies:

1. The total number of nodes adopted in the discretized model should obviously be minimized to enhance computation efficiency without jeopardizing accuracy. Thus, there is a need to develop a systematic method for optimally placing the elements in a horizon and also the nodes in each element.
2. Additional real-life case studies must be performed to further confirm the validity and usefulness of the proposed temporal flexibility analysis.

Acknowledgements

The authors wish to thank Prof. H. Chang and Prof. Y.H. Chen from Department of Chemical and Materials Engineering, Tamkang University, Taiwan for their useful suggestions in constructing the system model for SMDDS process.

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