Operating Strategies for Charging Batch Reactors under Multiple Constraints

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Effective strategies are proposed in this paper to carry out the critical tasks in charging batch reactors under multiple constraints. Specifically, a target-setting procedure is presented to achieve a desired level of reliability. A synthesis method for building the optimal alarm logic is also described in detail. The monitoring systems constructed according to this suggested approach are effective in reducing the probability of undetected faulty batches. These techniques have been tested with extensive simulation studies. The results show that the proposed strategies are suitable for application if high-value-added products are manufactured in the plant, which in fact is a prevailing situation of the batch processes.

Introduction

Batch processes have always been employed in the manufacture of small amounts of products with purities and/or other qualities not readily attainable in the continuous ones. In particular, specialty chemicals with high added value are often produced in batch reactors, e.g., specialty polymers, pharmaceuticals, biochemicals, etc. Since batch processing is time-variant in both operating conditions and system configuration, there is a need to place special emphasis on effective control in order to ensure operational safety and to achieve repeatable and accurate batches.

According to Perry *et al.* (1984), the operating sequence of a batch reactor typically consists of three stages, i.e., charging the reactor, manipulating the operating conditions to meet some processing criterion, and shutting down and emptying the reactor. To execute the operating procedure in each stage, the targets of control actions must be specified first. For example, the target amounts of the raw materials that must be charged into the reactor should be determined on the basis of production demand and/or some other operational constraints. Also, if an accurate mathematical model of the reaction system is available, the target profiles of the operating conditions can be established with the Pontryagin maximum principle (Cuthrell and Biegler, 1989; Villermaux and Georgakis, 1991).

In realistic operations, uncertainties and unexpected disturbances in the control actions are almost unavoidable. The above target-setting policies must thus be adjusted accordingly. Consequently, monitoring becomes another important control function. Most of the related studies in the past are concerned with the second stage of the batch reaction sequence. The task of monitoring is confined to checking that the planned operation steps are executed properly and that certain measurement variables are following predetermined trajectories *during* reaction. A detailed account of the literature can be found in Nomikos and MacGregor (1994). It should be noted that, in addition to the operating conditions during reaction, the outcome of a batch is sensitive to the initial state as well. For example, a runaway reaction may result from improper preparation of the raw materials, (Haldar and Rao, 1992). In other cases, the unreacted reactants remaining in the product may create undesirable downstream problems, such as separation difficulties, pollution, and safety hazards. Thus, it is clear that an accurate charging procedure, which includes a target-setting method and a monitoring scheme, is one of the primary factors for successful batch reactor control.

Despite the fact that various automatic batch chargers are available (Rosenof and Ghosh, 1987), the current target-setting practice in the industry is still experience-based. Furthermore, any inconsistency identified in the measurement data obtained from redundant sensors is usually resolved on the basis of operation experience. In a previous work, statistics-based strategies have been proposed for charging the batch reactors (Tsai and Chang, 1996). Specifically, various simple error models were first formulated according to the characteristics of different types of charging and measurement methods. On the basis of these models, several target-setting procedures were developed to achieve a given level of reliability and a systematic method for synthesizing the optimal alarm generation logic was also devised to minimize the expected loss due to misjudgments in monitoring.

Although effective, the above-mentioned strategies are in fact only suitable for processes with *one* operational constraint. Their applications are naturally quite limited. The objective of this study is thus to develop a more general solution to our problem. In particular, the target-setting procedure and the alarm-logic synthesis method have been modified to overcome the difficulties caused by the need to simultaneously satisfy multiple constraints. Descriptions of these improved strategies are presented in detail in this paper. An example is also provided to illustrate the implementation procedure of the proposed techniques. The feasibility and benefit of the present approach are demonstrated with extensive simulation results.

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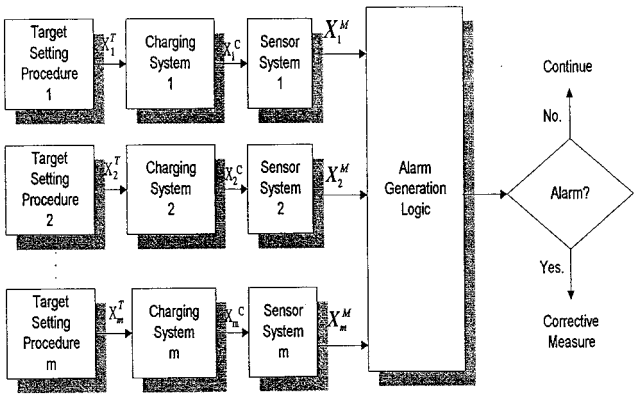

Figure 1. Charging operation of batch reactors.

Charging Operation of Batch Reactors

To avoid confusion, it is best to define the batch reactor charging process conceptually at the beginning of our argument. Figure 1 depicts the procedure of a typical charging operation associated with m reactants ($m \geq 1$). It is assumed that they can be fed simultaneously into the reactor. If more than m raw materials are involved, they are transferred separately according to Figure 1 in sequence.

Before the actual transfer takes place, the target amount X_i^{T} ($i = 1, 2, ..., m$) of each reactant, usually determined on the basis of market demand, must be given to the operator or specified in the computer program of PLC. These values can thus be regarded as constants during each batch. Each reactant is delivered from its storage tank either directly to the reactor or temporarily to a measure vessel first. The charge amount is manipulated manually or automatically according to the on-line measurements, e.g., readings of the level indicator on reactor or measure vessel, or the time elapsed since the inception of pumping operation. It should be noted that the amount of material *actually* charged into the reactor, i.e., X_i^{C} ($i = 1, 2, ..., m$), may not be exactly the same as its target. Both bias and random errors are possible in this transfer process. To ensure operational reliability and safety, it is a common industrial practice to install several independent and diversified sensors to monitor the actual charge amount of each reactant. Notice that in Figure 1 the output of a sensor system, say reactant i' ($1 \leq i' \leq m$), is represented with a vector $\mathbf{X}_{i'}^{\mathrm{M}} = [X_{i'}^{(1)}, X_{i'}^{(2)}, ..., X_{i'}^{(n_{i'})}]^{\mathrm{T}}$. There are a number of typical approaches available for measuring $X_{i'}^{\mathrm{C}}$, e.g., flow totalization of the raw material through the inlet pipeline and determination of the level change (by DP cell) or weight change (by weight cell) in the reactor or measure tank. Again, due to random and systematic errors, the measurement values of $X_{i'}^{\mathrm{C}}$, i.e., $X_{i'}^{(j)}$ ($j = 1, 2, ..., n_{i'}$), obtained from different sensors are, in general, not consistent with one another. Nonetheless, one is still required to check the status of the charging process against certain operational constraints with these data. Following is a general form of these constraints:

$$\Phi_k(X_1^{\mathrm{C}}, X_2^{\mathrm{C}}, ..., X_m^{\mathrm{C}}; Z_1^{\mathrm{C}}, Z_2^{\mathrm{C}}, ..., Z_n^{\mathrm{C}}) \geq 0 \qquad k = 1, 2, ..., N \tag{1}$$

where Z_j^{C} ($j = 1, 2, ..., n$) represents the actual amount of the jth raw material which has already been transferred into the reactor. In the study, Φ_k is referred to as the *performance function*. It is assumed that they are linear and also linearly independent. In other words, the rank of the coefficient matrix of Φ_k is N. For illustration convenience, a set of binary variables u_k are defined in this paper to represent the result of a reactor charging process:

$$u_k = \begin{cases} 1 & \text{if } \Phi_k < 0 \\ 0 & \text{if } \Phi_k \geq 0 \end{cases} \qquad k = 1, 2, ..., N \tag{2}$$

Usually, detection strategies for unacceptable conditions, i.e., the *alarm generation logic,* are developed on an *ad hoc* basis. For example, an alarm may be set off on the basis of the most reliable sensor or an arbitrarily chosen L-out-of-S ($L \leq S$ and S is the total number of independent methods for checking constraints) logic, etc. Once an alarm is generated, remedial measures should be taken to correct this undesirable condition. Otherwise, the subsequent steps specified in the operation manual can be executed in sequence.

Target-Setting Procedure

Owing to imperfect control and operation of the equipments, the actual amount of reactant charged into the reactor is usually not exactly the same as the target value, i.e.,

$$X_i^{\mathrm{C}} = X_i^{\mathrm{T}} + \Delta_i \qquad i = 1, 2, ..., m \tag{3}$$

where Δ_i is the error due to the charging system and, for convenience, it is assumed to be a normally distributed random variable. Two types of error models have been proposed in an earlier study (Tsai and Chang, 1996). For the sake of brevity, detailed descriptions of these model are omitted in the present paper. Notice also that, although both X_i^{C} and Δ_i are random variables, the target X_i^{T} should be viewed as a deterministic value in the charging process.

Because of charging errors, the plant engineers usually cannot guarantee the products of all batches in a production campaign to be satisfactory. Thus, the probability of operation failure can be considered as a performance index and chosen in advance. This performance index will be referred to as the *demand probability* in this paper. In practice, perfect operation cannot be expected; i.e., the demand probability should always be greater than zero. Since the performance functions Φ_k are functions of the random variables X_i^{C} and Z_j^{C}, the demand probability P_{F}, can be expressed as

$$P_{\mathrm{F}} = 1 - \int\int\int_D [\prod_{i=1}^{m} p_{X_i^{\mathrm{C}}}(\eta_i)] \times [\prod_{j=1}^{n} p_{Z_j^{\mathrm{C}}}(\xi_j)]\, \mathrm{d}\eta_1 \cdots \mathrm{d}\eta_m\, \mathrm{d}\xi_1 \cdots \mathrm{d}\xi_n \tag{4}$$

where $p_{X_i^{\mathrm{C}}}$ denotes the probability density function (pdf) of X_i^{C} and $p_{Z_j^{\mathrm{C}}}$ is the pdf of Z_j^{C}. The integration domain D in the above equation is the intersection of all constraints $\Phi_k \geq 0$ ($k = 1, 2, ..., N$) in the space formed by variables X_i^{C} ($i = 1, 2, ..., m$) and Z_j^{C} ($j = 1, 2, ..., n$).

Due to the fact that the value of $E[X_i^C]$ can be easily controlled by adjusting X_i^T, it is desirable to set the charge targets according to eq 4 so that a required level of demand probability P_F can be achieved. This task can always be accomplished as long as there is only one operational constraint. However, if more than one is involved in the charging process and $N > m$, it may not be possible to achieve any given level of performance. For example, D may be a closed region and thus the minimum achievable P_F may be significantly greater than zero. To limit the scope of this work, the present paper is only concerned with cases in which

$$m + n \geq N \tag{5}$$

From eq 5 and the fact that the performance functions are linearly independent, it is clear that the row vectors in the coefficient matrix of Φ_ks ($k = 1, 2, ..., N$) must span a N-dimensional subspace in the $(m + n)$-dimensional space formed by X_i^C s and Z_j^C s. Consequently, eq 4 can be written in an alternative form, i.e.

$$P_F = 1 - \int_0^\infty \int_0^\infty \cdots \int_0^\infty p_\Phi(\tau_1,\tau_2,...,\tau_N)\, d\tau_1\, d\tau_2 ... d\tau_N \tag{6}$$

where

$$\tau_k = \Phi_k(X_1^C,X_2^C,\cdots,X_m^C;Z_1^C,Z_2^C,\cdots,Z_n^C) \qquad k = 1, 2, ..., N \tag{7}$$

and p_Φ is the joint pdf of variables Φ_k ($k = 1, 2, ..., N$). Notice that, since P_F must be evaluated numerically, it is clearly easier to work with eq 6.

Optimal Alarm Generation Logic

As mentioned before, another important element in the charging operation of batch reactors is the monitoring scheme. It is assumed in this study that redundant sensors may be installed to measure the charge amount of the same reactant (see Figure 1). Let us consider the process of measuring X_i^C with sensor l ($l = 1, 2, ..., n_i$). Bias and random errors may both exist in this process. Thus

$$X_i^{(l)} = X_i^C + \Xi_i^{(l)} \qquad i = 1, 2, ..., m \qquad l = 1, 2, ..., n_i \tag{8}$$

where $\Xi_i^{(l)}$ is the measurement error associated with sensor l and it is also assumed to be normally distributed. In this study, it is further assumed that the charging errors Δ_i and these measurement errors $\Xi_i^{(l)}$ are statistically independent. The detailed descriptions of measurement error models can be found in Tsai and Chang (1996).

In order to determine the status of the current batch, on-line measurement data can be substituted into the performance functions Φ_k. Let us assume that S distinct sets of sensors are chosen for this purpose. For illustration convenience, these sets are collected in a sensor set M, i.e.

$$M = \{\mathbf{m}_s | \mathbf{m}_s = (i_1, i_2, ..., i_m; j_1, ..., j_n) \text{ and } s = 1, 2, ..., S\} \tag{9}$$

where $i_1, i_2, ..., i_m$ are the labels of the sensors for X_i^Cs, and $j_1, ..., j_n$ are the labels for Z_j^Cs. Corresponding to each $\mathbf{m}_s \in M$, the value of a binary indicator variable λ_{sk} can be determined, i.e.

$$\lambda_{sk} = \begin{cases} 1 & \text{if } \Phi_k^{(s)} < 0 \\ 0 & \text{otherwise} \end{cases} \qquad s = 1, 2, ..., S \qquad k = 1, 2, ..., N \tag{10}$$

where $\Phi_k^{(s)}$ is an *indicator function* whose value can be determined by substituting the s th set of measurement values into the performance function Φ_k, i.e.

$$\Phi_k^{(s)} = \Phi_k(X_1^{(i_1)},...,X_m^{(i_m)};Z_1^{(j_1)},...,Z_n^{(j_l)}) \tag{11}$$

$$i_1, ..., i_m, j_1, ..., j_l \in \mathbf{m}_s$$

and $X_1^{(i_1)}$, ..., $X_m^{(i_m)}$ and $Z_1^{(j_1)}$, ..., $Z_n^{(j_l)}$ are the on-line measurements of X_1^C, ..., X_m^C and Z_1^C, ..., Z_n^C respectively.

Notice that, in almost any traditional alarm system, only one operational constraint can be considered. However, since the N performance functions in eq 11 are correlated, it is not appropriate to install N separate alarms for the corresponding N constraints. Instead, a single system alarm should be generated on the basis of all indicator variables λ_{sk}. The logic for setting off the alarm can be explicitly expressed with an alarm function $f(\mathbf{\Lambda})$, i.e.

$$f(\mathbf{\Lambda}) = \begin{cases} 1 & \text{if the system is generating an alarm} \\ 0 & \text{otherwise} \end{cases} \tag{12}$$

where $\mathbf{\Lambda}$ is a $S \times N$ matrix and $\mathbf{\Lambda} = (\lambda_{sk})_{S\times N}$.

Obviously, the values of the indicator variables λ_{sk} may not be consistent with the true batch state after charging. There are two kinds of mistakes that can be identified accordingly, i.e., λ_{sk} is set to be 1 when $u_k = 0$ (type I mistake) and λ_{sk} is set to be 0 when $u_k = 1$ (type II mistake). Similarly, the mistakes committed in generating the *system alarm* can also be classified into types I and II. Since both types of mistakes result in financial losses, there are incentives for developing an optimal alarm generation logic which minimizes the expected loss Ψ, i.e.

$$\min_{f(\mathbf{\Lambda})} \Psi \tag{13}$$

where

$$\Psi = \sum_{\mathbf{\Lambda}} \{C_a(\mathbf{u})\, f(\mathbf{\Lambda}) + C_b(\mathbf{u})\, [1 - f(\mathbf{\Lambda})]\} Pr\{\mathbf{\Lambda},\mathbf{u}\} \tag{14}$$

where $C_a(\mathbf{u})$ and $C_b(\mathbf{u})$ respectively denote the losses caused by type I and II mistakes in alarm generation and $\mathbf{u} = [u_1, u_2, ..., u_N]^T$. The expected loss defined in eq 14 can also be written as:

$$\Psi = \sum_{\mathbf{u}} C_b(\mathbf{u})\, Pr\{\mathbf{u}\} - \sum_{\mathbf{\Lambda}} f(\mathbf{\Lambda})\, g(\mathbf{\Lambda}) \tag{15}$$

where

$$g(\mathbf{\Lambda}) = \sum_{\mathbf{u}} [C_b(\mathbf{u}) - C_a(\mathbf{u})] Pr\{\mathbf{\Lambda},\mathbf{u}\} \tag{16}$$

Notice that the first term on the right-hand side of eq 15 represents the expected loss of the no-sensor system. Thus, it is apparent that the expected loss is minimized

if the alarm function is chosen such that

$$f(\mathbf{\Lambda}) = \begin{cases} 1 & \text{if } g(\mathbf{\Lambda}) > 0 \\ 0 & \text{if } g(\mathbf{\Lambda}) \le 0 \end{cases} \tag{17}$$

After obtaining the values of $f(\mathbf{\Lambda})$ for all possible $\mathbf{\Lambda}$, its functional form can be constructed accordingly. With the functional form given, the logic associated with $f(\mathbf{\Lambda})$ can be implemented as a hard-wired circuit or as a computer program.

Finally, it should be pointed out that the sensor set M is not unique. Different combinations of s-independent sets $\mathbf{m}_s$ can be identified from the available sensors. Thus, the alarm logic is also affected by the sensors selected for determining the indicator variables λ_{sk} and the optimal system design should be obtained by

$$\min_{M_\kappa} \min_{f(\mathbf{\Lambda})} \Psi \tag{18}$$

where M_κ (κ = I, II, III, ...) denotes the κth sensor set.

Probability Evaluation

From eqs 16 and 17, it is clear that the joint probability $Pr\{\mathbf{\Lambda},\mathbf{u}\}$ must be evaluated in advance in order to implement the optimal alarm logic. Let us now consider the performance functions Φ_k and the indicator functions $\Phi_k^{(s)}$. They can be written in the following alternative forms:

$$\Phi_k = \Phi_k^{\mathrm{T}} + \Phi_{k,\Delta} \tag{19}$$

$$\Phi_k^{(s)} = \Phi_k + \Phi_{k,\Xi}^{(s)} = \Phi_k^{\mathrm{T}} + \Phi_{k,\Delta} + \Phi_{k,\Xi}^{(s)} \tag{20}$$

where

$$\Phi_k^{\mathrm{T}} = \Phi_k(X_1^{\mathrm{T}},X_2^{\mathrm{T}},...,X_m^{\mathrm{T}};Z_1^{\mathrm{T}},Z_2^{\mathrm{T}},...,Z_n^{\mathrm{T}}) \tag{21}$$

$$\Phi_{k,\Delta} = \Phi_k(\Delta_{X_1},\Delta_{X_2},...,\Delta_{X_m};\Delta_{Z_1},\Delta_{Z_2},...,\Delta_{Z_n}) - \Phi_{k,0} \tag{22}$$

$$\Phi_{k,\Xi}^{(s)} = \Phi_k(\Xi_1^{(i_1)},\Xi_2^{(i_2)},...,\Xi_{X_m}^{(i_m)};\Xi_{Z_1}^{(j_1)},\Xi_{Z_2}^{(j_2)},...,\Xi_{Z_n}^{(j_l)}) - \Phi_{k,0} \tag{23}$$

$$i_1, i_2, ..., i_m, j_1, j_2, ..., j_l \in \mathbf{m}_s$$

and

$$\Phi_{k,0} = \Phi_k(0,0,...,0;0,0,...,0) \tag{24}$$

Since Φ_ks and $\Phi_k^{(s)}$ s are linear functions of the normally-distributed charging errors and measurement errors, they should also be normally distributed random variables themselves. Thus, the joint probability $Pr\{\mathbf{\Lambda},\mathbf{u}\}$ can be determined by integrating the following pdf:

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{(N\times S+S)/2}|\mathbf{\Sigma}|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\mu)^{\mathrm{T}}\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu)\right] \tag{25}$$

where

$$\mathbf{x} = [\Phi_1^{(1)}, ..., \Phi_N^{(1)}, \Phi_1^{(2)}, ..., \Phi_N^{(2)}, ..., \Phi_1^{(S)}, ..., \Phi_N^{(S)}, \Phi_1, ..., \Phi_N]^{\mathrm{T}} \tag{26}$$

$$\mu = E[\mathbf{x}] \tag{27}$$

and $\mathbf{\Sigma}$ is the covariance matrix associated with $\mathbf{x}$. From the above formulations, it is clear that the computation demand is overwhelming if eq 25 is integrated directly. This situation is especially serious when the dimension of $\mathbf{x}$ becomes large. Consequently, there is a need to reduce the load in evaluating $Pr\{\mathbf{\Lambda},\mathbf{u}\}$ by making use of the fact that the sensors in $\mathbf{m}_s$ can be selected in such a way that the measurements corresponding to different sets are s-independent. In other words,

$$Pr\{\mathbf{\Lambda},\mathbf{u}\} = Pr\{\mathbf{\Lambda}|\mathbf{u}\}\, Pr\{\mathbf{u}\} = Pr\{\mathbf{u}\}\prod_{s=1}^{S} Pr\{\vec{\lambda}_s|\mathbf{u}\} \tag{28}$$

where

$$Pr\{\vec{\lambda}_s|\mathbf{u}\} = \frac{Pr\{\vec{\lambda}_s,\mathbf{u}\}}{Pr\{\mathbf{u}\}} \tag{29}$$

$$\vec{\lambda}_s = [\lambda_{s1}, \lambda_{s2}, ..., \lambda_{sN}] \tag{30}$$

and $s = 1, 2, ..., S$. Notice that the number of variables in $Pr\{\vec{\lambda}_s,\mathbf{u}\}$ is now reduced to $2N$.

An Application Example

The example presented here was designed to illustrate the implementation procedure of the proposed techniques. Since the actual amount of each reactant charged to the reactor is always unknown in practice and, also, there is an obvious need to quantify the benefits of adopting the present approach, a fictitious system is adopted in this paper for the purpose of producing simulated data.

Problem Statement. Let us consider a batch process in which the following reaction takes place:

$$\mathrm{A} + \mathrm{B} \rightarrow \mathrm{P} \tag{31}$$

where P is the batch product A and B are the reactants.

Let us further assume that reactant B is hazardous. Thus, the amount of B should be kept to a minimum after the batch reaction is terminated. One of the methods that can be adopted to achieve this purpose is to keep the feed ratio of A to B sufficiently high during the charging process. However, it is also obvious that the excess of reactant A initially charged to the reactor should not be too great. This is due to the need to avoid an unnecessary loss of raw material A.

On the basis of the above discussions, the first performance function in this example is assumed to be

$$\Phi_1(X_{\mathrm{B}}^{\mathrm{C}};Z_{\mathrm{A}}^{\mathrm{C}}) = bZ_{\mathrm{A}}^{\mathrm{C}} - aX_{\mathrm{B}}^{\mathrm{C}} - c \tag{32}$$

where Z_{A}^{C} represents the weight (in kilogram) of A which has already been charged to the reactor; $X_{\mathrm{B}}^{\mathrm{C}}$ denotes the weight (in kilogram) of B fed to the reactor in the present charging sequence; the values of constants a, b, and c are 0.007 188, 0.010 49, and 2.77, respectively.

Table 1. Means and Variances of Charging and Measurement Errors Associated with Reactants A and B

(a) Reactant A

	Z_A^δ	$\Xi_{ZA}^{(1)}$	$\Xi_{ZA}^{(2)}$	$Z_{A,\epsilon}^{(3)}$
mean	1.113	-2.423×10^2	5.8252×10^2	0.9658
variance	$5.365\ 87 \times 10^{-4}$	6.0225×10^4	$3.993\ 14 \times 10^4$	$2.588\ 13 \times 10^{-4}$

(b) Reactant B

	X_B^δ	$\Xi_{XB}^{(1)}$	$\Xi_{XB}^{(2)}$	$X_{B,\epsilon}^{(3)}$
mean	1.1310	-4.3240×10^2	7.5992×10^2	0.958235
variance	$2.594\ 57 \times 10^{-4}$	$4.305\ 96 \times 10^4$	$2.002\ 18 \times 10^4$	$1.131\ 03 \times 10^{-4}$

The second constraint in the charging operation is due to the processing capacity of the reactor. In other words, the total amount of reactants in the reactor should be kept below a predetermined upper limit. Thus, the second performance function used in this example is

$$\Phi_2 = -dZ_A^C - eX_B^C + f \tag{33}$$

where the values of constants d, e, and f are assumed to be 0.000 793 6, 0.000 398 4 and 18, respectively.

Error Models. It is assumed in this case that the charging errors associated with both A and B can be described with the following equations:

$$Z_A^C = Z_A^T\, Z_A^\delta = Z_A^T(1 + \delta_A) \tag{34}$$

$$X_B^C = X_B^T\, X_B^\delta = X_B^T(1 + \delta_B) \tag{35}$$

where Z_A^T and X_B^T denote the targets of reactants A and B, respectively, and Z_A^δ and X_B^δ are the random variables that account for the charging errors. Notice that δ_A and δ_B are also random variables and their means and variances are independent of the target values.

It is further assumed that three independent sensors are used for each reactant and the error models of the first two are

$$Z_A^{(i)} = Z_A^C + \Xi_{Z_A}^{(i)} \qquad i = 1, 2 \tag{36}$$

$$X_B^{(j)} = X_B^C + \Xi_{X_B}^{(j)} \qquad j = 1, 2 \tag{37}$$

where $\Xi_{Z_A}^{(i)}$ and $\Xi_{X_B}^{(j)}$ are the measurement errors associated with the ith sensor of reactant A and the jth sensor of reactant B, respectively.

Finally, the error models corresponding to the remaining sensors are assumed to be

$$Z_A^{(3)} = Z_A^C\, Z_{A,\epsilon}^{(3)} = Z_A^C(1 + \epsilon_A^{(3)}) \tag{38}$$

$$X_B^{(3)} = X_B^C\, X_{B,\epsilon}^{(3)} = X_B^C(1 + \epsilon_B^{(3)}) \tag{39}$$

where $Z_{A,\epsilon}^{(3)}$ and $X_{B,\epsilon}^{(3)}$ are the random variables that account for the measurement errors. Similarly, the means and variances of the random variables $\epsilon_A^{(3)}$ and $\epsilon_B^{(3)}$ are assumed to be independent of their respective true values, i.e., Z_A^C and X_B^C.

In order to simulate the batch charging process with a random number generator, the means and variances of the random variables in the error models must be specified. These data are provided in Table 1a,b. In realistic operation, the statistics of the charging and measurement errors must be obtained from historical data. Using subroutine DRNNOA in IMSL (Kinderman and Ramage, 1976), these data have been created according to the targets specified for each batch and the parameters listed in Table 1a,b. A total of 320 "previous" batches have been simulated in this example.

By making use of the techniques suggested by Tsai and Chang (1996), the variances of all measurement errors can be estimated first. Then, maximum likelihood estimates of the rest of the parameters associated with the charging and measurement errors can be determined accordingly. The results of this iterative calculation are presented in Table 2a,b.

Target Setting Procedures. Having obtained the estimated parameters, one can then compute the charging targets for "future" batches. It should be noted that eq 6 is the foundation of the targeting procedure. In the present example, this equation is

$$P_F = 1 - \int_0^\infty \int_0^\infty p_\Phi(\tau_1,\tau_2)\, d\tau_1\, d\tau_2 \tag{40}$$

The means associated with the pdf p_Φ are

$$E[\Phi_1] = bZ_A^T E[Z_A^\delta] - aX_B^T E[X_B^\delta] - c \tag{41}$$

$$E[\Phi_2] = -dZ_A^T E[Z_A^\delta] - eX_B^T E[X_B^\delta] + f \tag{42}$$

The variances and covariances in the covariance matrix of p_Φ can be written as

$$\mathrm{Var}[\Phi_1] = (bZ_A^T)^2 \mathrm{Var}[Z_A^\delta] + (aX_B^T)^2 \mathrm{Var}[X_B^\delta] \tag{43}$$

$$\mathrm{Var}[\Phi_2] = (dZ_A^T)^2 \mathrm{Var}[Z_A^\delta] + (eX_B^T)^2 \mathrm{Var}[X_B^\delta] \tag{44}$$

$$\mathrm{Cov}[\Phi_1,\Phi_2] = ae(X_B^T)^2 \mathrm{Var}[X_B^\delta] - bd(Z_A^T)^2 \mathrm{Var}[Z_A^\delta] \tag{45}$$

Based on the estimates of $E[Z_A^\delta]$, $E[X_B^\delta]$, $\mathrm{Var}[Z_A^\delta]$, and $\mathrm{Var}[X_B^\delta]$ listed in Table 2a,b, eq 40 can be solved iteratively with the subroutine DQAND in IMSL to determine target X_B^T for use throughout the production campaign according to a set of given Z_A^T and P_F. In this case, these two values were chosen to be 12 046.6 kg (Z_A^T) and 0.05 (P_F), and the resulting target for B was $X_B^T = 15\ 421$ kg.

In order to quantitatively demonstrate the advantages of our approach, additional simulation studies have been carried out. A total of 4096 batches were simulated to verify the correctness of the above results. It was found that the proportion of failed batches is about 4.57%, which is fairly close to the assigned value. A sample of the simulation results is shown in Figure 2a,b. Notice that the points under the horizontal line in each figure represent failed batches.

Optimal Alarm Logics. As mentioned before, the outcome of reactant-charging operation can be monitored with on-line sensors. All possible sensor sets used in the present example are listed in Table 3. Notice that

Table 2. Estimated Means and Variances of Charging and Measurement Errors Associated with Reactants A and B

(a) Reactant A

	Z_A^{δ}	$\Xi_{ZA}^{(1)}$	$\Xi_{ZA}^{(2)}$	$Z_{A,\epsilon}^{(3)}$
estimated mean	1.104 12	$-2.290\ 49 \times 10^2$	$6.150\ 26 \times 10^2$	0.966 527
estimated variance	$5.937\ 96 \times 10^{-4}$	$6.220\ 27 \times 10^4$	$4.406\ 47 \times 10^4$	2.371×10^{-4}

(b) Reactant B

	X_B^{δ}	$\Xi_{XB}^{(1)}$	$\Xi_{XB}^{(2)}$	$X_{B,\epsilon}^{(3)}$
estimated mean	1.132 58	$-4.681\ 79 \times 10^2$	$7.506\ 52 \times 10^2$	0.957 283
estimated variance	$2.418\ 19 \times 10^{-4}$	$4.417\ 78 \times 10^4$	$2.164\ 47 \times 10^4$	$1.118\ 71 \times 10^{-4}$

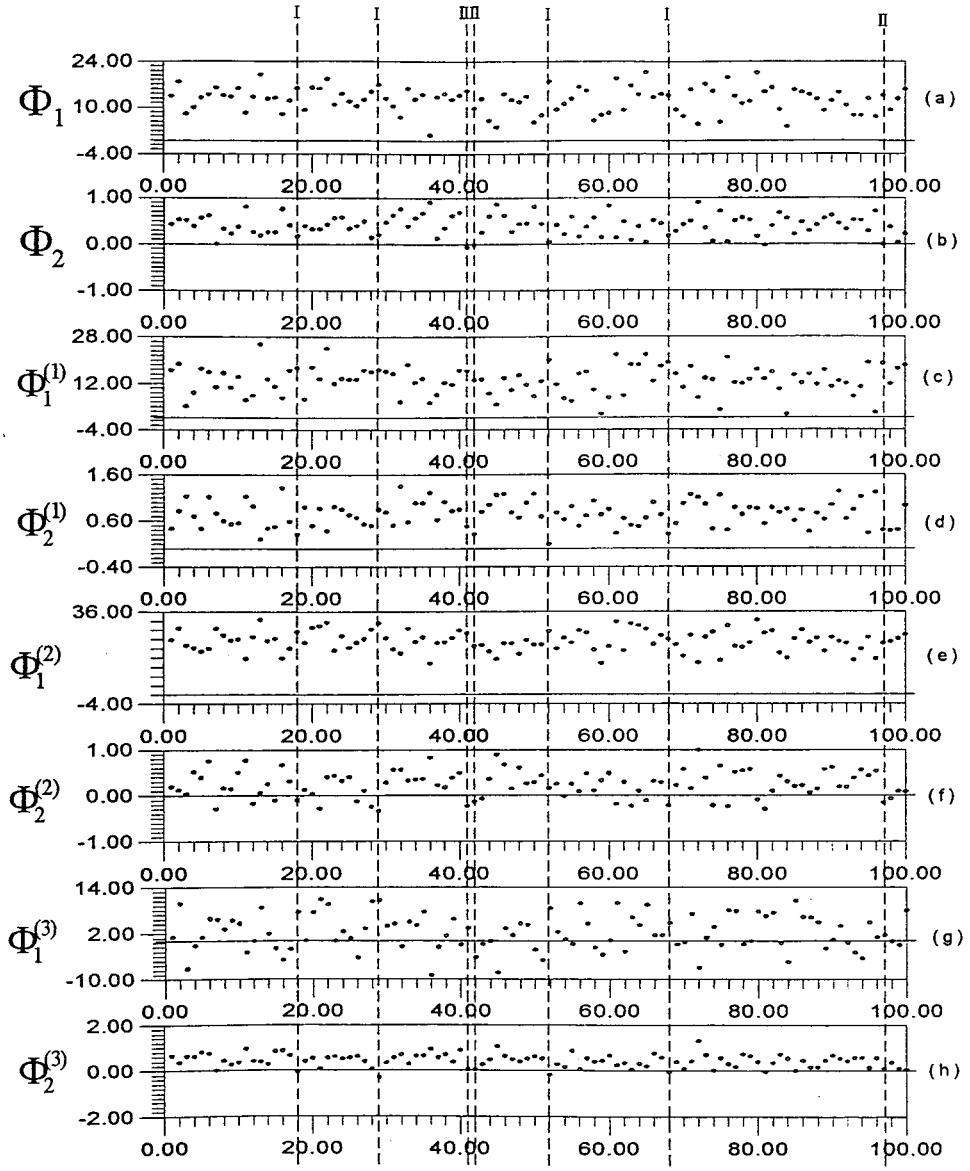

Figure 2. Sample of the simulation results obtained with the target setting strategy ($P_F = 0.05$) and optimal alarm logic: (a) actual values of the performance function Φ_1; (b) actual values of the performance function Φ_2; (c) values of the indicator function $\Phi_1^{(1)}$; (d) values of the indicator function $\Phi_2^{(1)}$; (e) values of the indicator function $\Phi_1^{(2)}$; (f) values of the indicator function $\Phi_2^{(2)}$; (g) values of the indicator function $\Phi_1^{(3)}$; (h) values of the indicator function $\Phi_2^{(3)}$.

the sets $\mathbf{m}_s$ ($s = 1, 2, 3$) within each sensor set M_κ ($\kappa =$ I, II, ..., VI) are chosen in such a way that, corresponding to each reactant, any sensor label appears only once. Consequently, the resulting indicator values λ_{sk} ($s = 1, 2, ..., S$) of a given performance function Φ_k ($k = 1$ or 2) should be statistically independent. Also notice that the task of constructing alarm generation logic is essentially equivalent to that of determining the form of the alarm function $f(\mathbf{\Lambda})$. To achieve this purpose, one can conclude from eqs 16 and 17 that the values of $Pr\{\mathbf{\Lambda},\mathbf{u}\}$ corre-

Table 3. Sensor Sets

	κ					
s	I	II	III	IV	V	VI
1	(1,1)	(1, 1)	(1, 2)	(1, 2)	(1, 3)	(1, 3)
2	(2, 2)	(2, 3)	(2, 1)	(3, 1)	(2, 2)	(3, 2)
3	(3, 3)	(3, 2)	(3, 3)	(2, 3)	(3, 1)	(2,1)

Table 4. Costs of Type I and II Mistakes

u_1	u_2	C_a	C_b
0	0	1.0	0.0
1	0	0.0	40.0
0	1	0.0	20.0
1	1	0.0	80.0

Table 5. Minimum Expected Losses

	κ					
	I	II	III	IV	V	VI
Ψ/C_a	0.962 63	0.957 37	0.961 95	0.959 89	0.962 63	0.963 00

sponding to all combinations of $\mathbf{\Lambda}$ and $\mathbf{u}$ must be evaluated first. In this example, these probabilities were evaluated according to eqs 28−30. Again, the corresponding computations can be carried out with subroutine DQAND in IMSL. The estimates in Table 2a,b were used to estimate the parameters in the pdf's $p(\vec{\lambda}_s,\mathbf{u})$ and $p(\mathbf{u})$.

Corresponding to a demand probability of 0.05, the targets of reactants A and B have already been determined previously, i.e., $Z_A^T = 12\,046.6$ kg and $X_B^T = 15\,421$ kg. In this example, the losses caused by type I and II mistakes are assumed to be the ones listed in Table 4. On the basis of these assumptions and the joint probabilities determined with eqs 28−30, the minimum expected losses associated with all sensor sets listed in Table 3 can be calculated with eqs 15−17 (see Table 5). The best sensor set among the six possible candidates can then be selected accordingly. From Table 5, it is apparent that M_{II} should be our choice. The corresponding alarm function $f(\mathbf{\Lambda})$ can be determined by computing function $g(\mathbf{\Lambda})$ with eq 16. To save space, the optimal alarm function corresponding to sensor set M_{II} is presented here with the following notation:

$$f(\lambda_{11},\lambda_{12},\lambda_{21},\lambda_{22},\lambda_{31},\lambda_{32}) \leftrightarrow \begin{Bmatrix} 0&1&0&1&0&1&0&1\\ 0&1&0&1&0&1&1&1\\ 1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1\\ 1&1&1&1&0&1&1&1\\ 0&1&0&1&0&1&1&1\\ 1&1&1&1&1&1&1&1\\ 1&1&1&1&1&1&1&1 \end{Bmatrix} \quad (46)$$

The values of the alarm function $f(\mathbf{\Lambda})$ corresponding to 64 combinations of $\mathbf{\Lambda}$ are all given in eq 46. The position (p, q) of each entry in the array is related to a particular set of λ_{ij}s. Specifically, the following relation can be utilized:

$$8(p-1)+q-1 = \lambda_{11}\times 2^5 + \lambda_{12}\times 2^4 + \lambda_{21}\times 2^3 + \lambda_{22}\times 2^2 + \lambda_{31}\times 2^1 + \lambda_{32}\times 2^0 \quad (47)$$

For example, let us consider the entry at position (1, 3). Since $8(1-1)+3-1=2$ and the corresponding binary number is 10, the alarm function should therefore be

$$f(0,0,0,0,1,0) = 0 \quad (48)$$

Extensive numerical simulation studies have also been carried out to test this alarm logic. The simulated data of Z_A^C and X_B^C, which were used for evaluating the performance of target-setting procedures (Figure 2a,b), were again adopted for the present purpose. The measurement errors were also simulated with a random number generator according to the parameters listed in Table 2a,b. The measurement data were then produced by adding the actual charge amounts and corresponding measurement errors. A sample of the results is presented in Figure 2c−h. Notice that the failed batches corresponding to type I and II mistakes are marked with dashed lines in these figures. It was found in our simulation that the percentage of the former is about 3.418% and that of the latter is 2.344%.

It should be noted that, without implementing the alarm logic, only type II mistakes are possible in the charging operation. The corresponding probability is essentially the demand probability P_F. Thus, one can clearly observe that the alarm system can affect the batch reaction process in two different ways. Certainly, the major advantage of alarm is that the probability of type II mistakes can be further reduced. On the other hand, it also causes a loss due to type I mistakes.

Suboptimal Coherent Alarm Logics. It should be noted that the optimal alarm logic presented in eq 46 is, in fact, *incoherent*. In particular, the requirement of a *non-negative contribution* is usually imposed on an alarm system, i.e.

$$\mathbf{\Lambda} \le \tilde{\mathbf{\Lambda}} \Rightarrow f(\mathbf{\Lambda}) \le f(\tilde{\mathbf{\Lambda}}) \quad (49)$$

This requirement is clearly violated in several cases. For example, eq 46 implies not only

$$f(1,0,0,0,0,0) = 1 \quad (50)$$

but also

$$f(1,0,0,1,0,0) = 0 \quad (51)$$

$$f(1,0,1,0,0,0) = 0 \quad (52)$$

$$f(1,0,1,0,1,0) = 0 \quad (53)$$

$$f(1,0,1,1,0,0) = 0 \quad (54)$$

Thus, although eq 46 is practically implementable, it is still desirable to develop a logic design which is coherent and, at the same time, almost optimal. Two candidates have been identified. The first is obtained by changing the entries at positions (5, 1), (5, 3), and (5, 7) in eq 46 from 1 to 0. The resulting alarm function can then be represented by

$$f(\lambda_{11},\lambda_{12},\lambda_{21},\lambda_{22},\lambda_{31},\lambda_{32}) = 1 - (1-\lambda_{32})(1-\lambda_{12})(1-\lambda_{21}\lambda_{22}\lambda_{31}) \quad (55)$$

The corresponding increase in expected loss is approximately 4.4×10^{-5}.

The second suboptimal coherent logic can be produced by changing the entries at positions (5, 5), (6, 1), (6, 3),

and (6, 5) from 0 to 1. Consequently, the alarm function becomes

$$f(\lambda_{11},\lambda_{12},\lambda_{21},\lambda_{22},\lambda_{31},\lambda_{32}) = 1 - (1-\lambda_{11})(1-\lambda_{12})(1-\lambda_{32})(1-\lambda_{21}\lambda_{22}\lambda_{31}) \quad (56)$$

The increase in Ψ is now 2.9×10^{-5}. Simulation studies have also been carried out to test the alarm logic given in eq 56. It was found that the percentage of type I failures is about 3.419% and that of type II is 2.34%. Thus, for all practical purposes, the effectiveness of the suboptimal logic is the same as that of an optimal one.

Conclusions

Several statistical operating strategies have been developed in this study for charging the batch reactors under multiple constraints. The target-setting procedure can be implemented to achieve a given level of reliability. The suboptimal coherent alarm generation system can be installed to reduce the probability of undetected charge failures. The results of implementing the suggested strategies to the application example show that the approach taken in this study is feasible and effective. Further, when compared with the current practice in the industry, these strategies are superior under the condition that a higher-value-added product is produced in the process.

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Nomenclature

C_a: financial loss resulting from type I mistakes
C_b: financial loss resulting from type II mistakes
$E[\cdot]$: mean operator
$f(\cdot)$: alarm function
m: number of reactants being charged simultaneously in the current operation
n: number of reactants which have already been charged in the current batch
N: number of operational constraints
n_i: total number of senosrs used for monitoring the reactant i
$p(\cdot)$: probability density function
P_F: demand probability
u_k: binary indicator variable for $\Phi_k(\cdot)$
Var[·]: variance operator
X_i^C: amount of reactant i actually charged into the reactor
$X_i^{(l)}$: measurement of X_i^C from the lth sensor
X_i^T: target of X_i^C
Z_j^C: actual amount of the j th reactant which has already been charged
$Z_j^{(n)}$: measurement of Z_j^C obtained from the nth sensor
Z_j^T: target of Z_j^C

Greek Symbols

λ_{sk}: binary indicator variable for $\Phi_k^{(s)}(\cdot)$
Δ_i: charging error of reactant i
$\Xi_i^{(l)}$: measurement error of reactant i associated with sensor l
$\Phi_k(\cdot)$: kth performance function
$\Phi_k^{(s)}(\cdot)$: sth indicator function associated with $\Phi_k(\cdot)$
Ψ: expected loss due to failed operation

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