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A STATISTICS BASED APPROACH TO ENHANCING SAFETY AND RELIABILITY OF THE BATCH-REACTOR CHARGING OPERATION

CHII-SHANG TSAI and CHUEI-TIN CHANG

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

Abstract - In general there are two critical decisions that must be made in the charging sequence of batch reactors, i.e. target setting and alarm generation. In this paper, a number of statistics-based strategies are proposed to perform these tasks. Specifically, both off-line and on-line target setting procedures are presented and either one of them can be adopted to increase the profit margin of any given batch process without sacrificing reliability. A synthesis method for building 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 batch processes.

THE 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. Fig. 1 depicts the procedure of a typical charging operation associated with one reactant. If more than one raw material are involved, they are fed separately according to Fig. 1 in sequence.

Before the actual transfer takes place, a target amount X^t, usually determined on the basis of market demand, must be given to the operator or specified in the computer program of PLC (Crooks et al., 1992). This value can thus be regarded as a known constant during each batch. In order to ensure operational reliability and safety, it is a common practice to install several independent and diversified sensors for monitoring purpose (Rosenof and Ghosh, 1987). It should be noted that the amount of material *actually* charged into the reactor, i.e. X^c, may not be exactly the same as the target and in general should be different from the measurement values. Both bias and random errors occur in the the charging and measuring processes.

In practice, inequality constraints are often imposed to address safety concerns. These constraints are written here in a generalized form with *performance functions* $\mathcal{G}$, i.e.

$$\mathcal{G}(X^c; Z_1^c, \ldots, Z_N^c) \geq 0 \tag{1}$$

where Z_j^c represents the actual amount of the jth *raw material* and which has already been transferred into the reactor.

ERROR MODELS

To understand the nature of our problems at hand, it is necessary to gain a clear picture of the errors associated with the charging and measuring processes. Let us first consider the process of charging. Owing to imperfect control and operation of the equipments, the actual amount of reactant charged into reactor is usually not exactly the same as the target value, i.e.

$$X^c = X^t + \Delta \tag{2}$$

where, Δ is the error due to the charging system and, for convenience, it is assumed to be a normally distributed random variable. Notice that, although both X^c and Δ are random variables, the target X^t should be viewed as a deterministic value in the charging process. The simplest approach to describe the

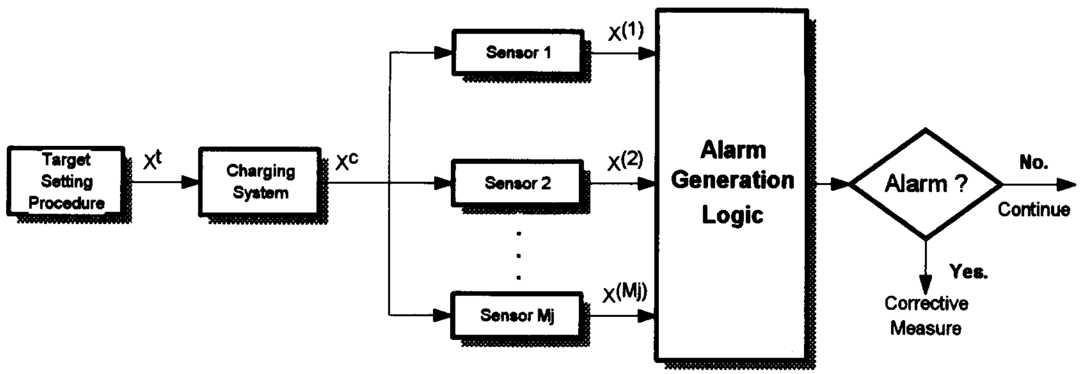

Fig. 1. The Charging Operation of Batch Reactors.

behavior of Δ is to assume that it is independent of the target amount. This assumption is reasonable if the charging process is stopped on the basis of level or weight measurements. Throughout this paper, these errors will be referred to as the *charging errors of type A*. The second approach adopted in this study is to assume that the charging error is proportional to the targeted amount, i.e.

$$\Delta = X^t \delta \tag{3}$$

where the mean and variance of δ are not affected by X^t. From a practical viewpoint, these charging errors exist when the transferring flow is maintained and terminated according to flow measurements. Errors that can be described by Eq.(3) are called *charging errors of type B* in this study.

Next, let us consider the process of measuring X^c with sensor i ($i = 1, 2, \cdots, M$). Bias and random errors may both exist in this process. The measurement errors are again described with two similar models. *Measurement errors of type A* refers to errors not affected by X^c. Thus,

$$X^{(i)} = X^c + \Xi^{(i)} \tag{4}$$

where $X^{(i)}$ and $\Xi^{(i)}$ denote respectively the measurement value and error associated with sensor i and the latter is also assumed to be normally distributed (Gupta and Narasimhan, 1993). In addition, the corresponding mean $E\left[\Xi^{(i)}\right]$ and variance $\mathrm{Var}\left[\Xi^{(i)}\right]$ should be independent of the actual charge amount X^c. On the other hand, if $\Xi^{(i)}$ in Eq.(4) is *of type B*, it should be written as

$$\Xi^{(i)} = X^c \epsilon^{(i)} \tag{5}$$

Finally, it is assumed that the errors Δ and $\Xi^{(i)}$s are statistically independent.

Since the statistics-based techniques are probably the most appropriate tools for the development of a target setting procedure and to devise the alarm generation logic, the parameters that describe the probability distributions of charging and measurement errors must first be estimated correctly. Although, in principle, the maximum likelihood estimates of parameters can be obtained with a standard algorithm, the computational load is usually extremely demanding. Simplification techniques have been developed in this study to enhance computation efficiency. A detailed description of these techniques can be found in Tsai and Chang (1995).

THE ON-LINE TARGET SETTING STRATEGY

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 successful charging operation, i.e. reliability, can be considered as a performance index and should be chosen in advance. In practice, perfect operation cannot be expected, i.e. the achievable reliability should be always less than one.

As long as an operational constraint can be defined for the charging process, any given level of performance can be achieved with a proper target setting procedure. Since the performance function $\mathcal{G}$ is a function of random variables X^c and Z_j^cs, the probability of $\mathcal{G} < 0$, i.e. the demand probability P_F, can be expressed as

$$P_F = 1 - \int_0^{\infty} f_{\mathcal{G}}(\eta)d\eta = 1 - \int_{-\gamma}^{\infty} \tilde{f}_{\tilde{\mathcal{G}}}(\xi)d\xi \tag{6}$$

where,

$$\tilde{\mathcal{G}} = \frac{\mathcal{G} - E[\mathcal{G}]}{\sqrt{\text{Var}[\mathcal{G}]}} \quad \text{and} \quad \gamma = \frac{E[\mathcal{G}]}{\sqrt{\text{Var}[\mathcal{G}]}} \tag{7}$$

and $f_{\mathcal{G}}$ and $\tilde{f}_{\tilde{\mathcal{G}}}$ are the probability density functions of $\mathcal{G}$ and $\tilde{\mathcal{G}}$ respectively. The lower bound of the integral in Eq.(6), i.e. γ, will later be referred to as the *safety index* (Kapur and Lamberson, 1991).

Notice that both X^c and Z_j^c ($j = 1, 2, \ldots, N$) are functions of the charging errors only and, also, these errors are assumed to follow Gaussian distribution in this study. If the performance function is a linear function of X^c and Z_j^cs, then $\mathcal{G}$ must also be normally distributed. However, if the performance function is nonlinear, the value of safety index can still be approximated using linearization techniques (Tsai and Chang, 1995).

Since the value of $E[\mathcal{G}]$ can be manipulated by adjusting X^t and Z_j^ts, it is convenient to set the charge targets *off-line* according to Eqs.(7) so that a required level of P_F can be achieved. However, if this approach is taken, the corresponding target setting procedure tends to be conservative. This is due to the fact that variabilities associated with X^c and Z_j^cs must both be accounted in estimating $\text{Var}[\mathcal{G}]$.

One of the *on-line* approaches used in this study is to obtain least square estimates of Z_j^c based on measurements of the *current* batch, i.e.

$$\hat{Z}_j^c = \left(\sum_{i=1}^{M_j} \frac{\bar{Z}_j^{(i)} - E\left[\Xi_{Z_j}^{(i)}\right]}{\text{Var}\left[\Xi_{Z_j}^{(i)}\right]} \right) \Big/ \left(\sum_{i=1}^{M_j} \frac{1}{\text{Var}\left[\Xi_{Z_j}^{(i)}\right]} \right) \tag{8}$$

where, M_j is the number of sensors used for Z_j^c and $\bar{Z}_j^{(i)}$ denotes the current measurement value of the ith sensor. The means and variances of the corresponding estimation errors, d_j, can be shown to be

$$E\left[d_j\right] = 0 \quad \text{and} \quad \text{Var}\left[d_j\right] = \left(\sum_{i=1}^{M_j} \frac{1}{\text{Var}[\Xi_{Z_j}^{(i)}]} \right)^{-1} \tag{9}$$

THE OPTIMAL ALARM GENERATION LOGIC

As mentioned before, multiple sensors are usually used to monitor the charging sequence. 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 $\mathcal{M}$, i.e.

$$\mathcal{M} = \{\mathbf{m}_s \mid \mathbf{m}_s = (i, j_1, \cdots, j_N) \text{ and } s = 1, 2, \cdots, S\} \tag{10}$$

where i, j_1, ..., j_N are the labels of the sensors for X^C, Z_1^C, ..., Z_N^C respectively. Corresponding to each $\mathbf{m}_s \in \mathcal{M}$, the value of a binary indicator variable y_s can be determined, i.e.

$$y_s = \begin{cases} 1 & \text{if } \mathcal{G}^{(s)} < 0 \\ 0 & \text{otherwise} \end{cases} \tag{11}$$

where, $s = 1, 2, \cdots, S$. $\mathcal{G}^{(s)}$ is an *indicator function* whose value can be determined by substituting the sth set of measurement values into the performance function. The system alarm can then be generated on the basis of these indicators. The logic for setting off the alarm can be explicitly expressed with an alarm function $f(\mathbf{y})$, i.e.

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

where $\mathbf{y} = [y_1, y_2, \cdots, y_S]^T$. Obviously, the values of the indicator variables y_ss may not be consistent with the true batch state after charging. Specifically, let us consider the true value of the performance function, i.e.

$$\mathcal{G}^c = \mathcal{G}(X^c; Z_1^c, Z_2^c, \cdots, Z_N^c) \tag{13}$$

There are two kinds of mistakes that can be identified accordingly, i.e. y_s is set to be 1 when $\mathcal{G}^C \geq 0$ (type I mistake) or y_s is set to be 0 when $\mathcal{G}^C < 0$ (type II mistake). Similarly, the mistakes committed in generating the *system alarm* can also be classified into type I and II. The conditional probabilities associated with these two mistakes, i.e. P_a and P_b, can be expressed as

$$P_a = Pr\left\{f(\mathbf{y}) = 1 \mid \mathcal{G}^C \geq 0\right\} = \sum_{\mathbf{y}} f(\mathbf{y}) Pr\left\{\mathbf{y} \mid \mathcal{G}^C \geq 0\right\} \tag{14}$$

$$P_b = Pr\left\{f(\mathbf{y}) = 0 \mid \mathcal{G}^C < 0\right\} = \sum_{\mathbf{y}} [1 - f(\mathbf{y})] Pr\left\{\mathbf{y} \mid \mathcal{G}^C < 0\right\} \tag{15}$$

Since both types of mistakes result in financial losses, there are incentives for developing an optimal alarm generation logic which minimizes the expected loss $\mathcal{L}$, which its definition is defined as

$$\mathcal{L} = C_a(1 - P_F)P_a + C_b P_F P_b \tag{16}$$

$$= C_b P_F - \sum_{\mathbf{y}} f(\mathbf{y}) h(\mathbf{y}) \tag{17}$$

where C_a and C_b respectively denote the losses caused by type I and II mistakes in alarm generation. The function $h(\mathbf{y})$ is

$$h(\mathbf{y}) = C_b P_F Pr\left\{\mathbf{y} \mid \mathcal{G}^C < 0\right\} - C_a(1 - P_F) Pr\left\{\mathbf{y} \mid \mathcal{G}^C \geq 0\right\} \tag{18}$$

Thus, it is apparent that the expected loss is minimized if the alarm function is chosen such that $f(\mathbf{y}) = 1$ for $h(\mathbf{y}) > 0$ and 0 for $h(\mathbf{y}) \leq 0$.

A CASE STUDY

In this example, a simple reaction, i.e. $a'\mathcal{A} + b'\mathcal{B} \longrightarrow Product$, is considered. The constraint of charging operation is to ensure complete conversion of one of the reactants, say $\mathcal{B}$. Component $\mathcal{A}$ is assumed to be charged first. Thus, the performance function can be written as

$$\mathcal{G} = bZ_{\mathcal{A}}^c - aX_{\mathcal{B}}^c - c \tag{19}$$

where, $Z_{\mathcal{A}}^c$ and $X_{\mathcal{B}}^c$ are the weight (kg) of $\mathcal{A}$ and $\mathcal{B}$ actually charged to the reactor and c is a constant which takes into account of the effects of minor side reactions. The constants a, b and c are assumed to be 0.007188, 0.01049 and 2.77 respectively.

Let us further assume that the charging system of this reactor can be described by the simplified flow diagram presented in Fig. 2. Specifically, the transferring flow is assumed to be maintained and terminated according to flow measurements. The charge amounts of $\mathcal{A}$ and $\mathcal{B}$ are monitored with level transducers in the storage tanks and the reactor (sensor #1 and #2) and a flow totalizer on the inlet pipeline (sensor #3).

Error Models — In the present case, the charging errors of both $\mathcal{A}$ and $\mathcal{B}$ are assumed to be *of type B*. The measurement errors associated with the first two sensors of both components are *of type A*. Those corresponding to the rest are *of type B*.

Parameter Estimation — In realistic operation, the statistics of the charging and measurement errors must be obtained from historical data. Simulated data are used instead in this example for illustration purpose. Using subroutine DRNNOA in IMSL (Kinderman and Ramage, 1976), normally-distributed data have been created according to the targets specified for each batch and the parameters listed in the following two tables. A total of 320 "previous" batches have been simulated.

parameters	δ_{Z_A}	$\Xi_{Z_A}^{(1)}$	$\Xi_{Z_A}^{(2)}$	$\epsilon_{Z_A}^{(3)}$
bias	0.113	-2.423×10^2	5.8252×10^2	−0.034191
variance	5.36587×10^{-4}	6.0225×10^4	3.99314×10^4	2.58813×10^{-4}

parameters	δ_{X_B}	$\Xi_{X_B}^{(1)}$	$\Xi_{X_B}^{(2)}$	$\epsilon_{X_B}^{(3)}$
bias	0.131	-4.324×10^2	7.5992×10^2	−0.041765
variance	2.59457×10^{-4}	4.30596×10^4	2.00218×10^4	1.13103×10^{-4}

Then, maximum likelihood estimates associated with the charging and measurement errors can be de-

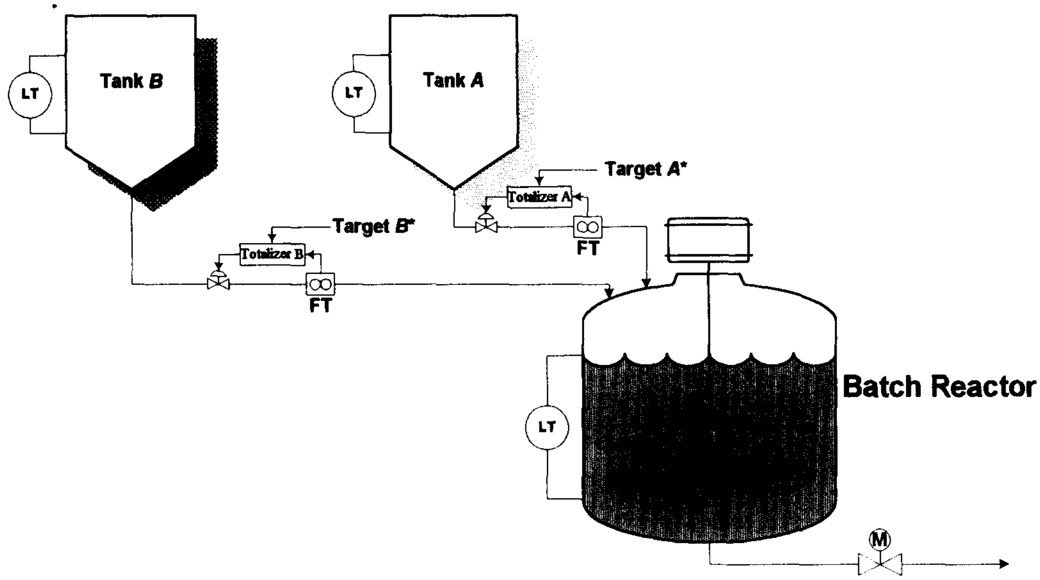

Fig. 2. A schematic diagram of a batch reactor.

termined accordingly. The results of the iterative calculation are presented in the following two tables.

parameters	δ_{Z_A}	$\Xi^{(1)}_{Z_A}$	$\Xi^{(2)}_{Z_A}$	$\epsilon^{(3)}_{Z_A}$
bias	0.10412	-2.29049×10^2	6.15026×10^2	-0.033473
variance	5.93796×10^{-4}	6.22027×10^4	4.40647×10^4	2.37100×10^{-4}

parameters	δ_{X_B}	$\Xi^{(1)}_{X_B}$	$\Xi^{(2)}_{X_B}$	$\epsilon^{(3)}_{X_B}$
bias	0.13258	-4.68179×10^2	7.50652×10^2	-0.042717
variance	2.41819×10^{-4}	4.41778×10^4	2.16447×10^4	1.11871×10^{-4}

From these results, one can see that the estimation accuracy is in general acceptable.

Off-Line Setting Strategy — Without evaluating the actual charge amount of $\mathcal{A}$ in every batch, Eq.(7) can be solved in advance to determine a constant $X^t_{\mathcal{B}}$ for use throughout the production campaign according to a set of given values of $Z^t_{\mathcal{A}}$ and γ. For example, the value of $X^t_{\mathcal{B}}$ corresponding to $P_F = 10^{-6}$ can be determined to be 16239.0 kg. On the other hand, if the profit of producing more product per batch is quite high and the loss due to improper charging operation is not overwhelming, there may be incentives to accept a higher demand probability. As another example, the target for reactant $\mathcal{B}$ can be raised to 17438.0 kg if $P_F = 0.05$. This change represents a 5.7% increase in productivity.

The correctness of the proposed target setting procedure has been verified in our studies, which included 1024 batches with the same target for reactant A, i.e. $Z^t_{\mathcal{A}} = 13046.6$ kg. The percentage of failed batches in the former example was found to be around 5.1%, which is very close to the target value of $P_F = 0.05$.

On-Line Setting Strategy — The simulation data of reactant $\mathcal{A}$ used in the this case were essentially the same as those adopted for testing the off-line strategy. Having obtained the simulated on-line measurements of $\mathcal{A}$, the value of $\hat{Z}^c_{\mathcal{A}}$ was estimated in every batch according to Eq.(8). Using a demand probability of 0.05, the target of reactant $\mathcal{B}$ for every batch was then determined by solving Eq.(7). Finally, the simulated data of reactant B were produced with a random number generator. The percentage of failed batches was again found to be very close to the target demand probability. Its value is approximately 4.92% this time. A sample of the simulation results for this case is provided in Fig. 3.

It should also be noted that the average value of $X^t_{\mathcal{B}}$ now can be raised to 17735.2 kg. This result shows that, when compared with the off-line strategy, the profit margin of the batch process can be increased with the on-line approach while still maintaining the same target demand probability.

The Alarm Generation Logic — As mentioned before, the outcome of reactant-charging operation can be

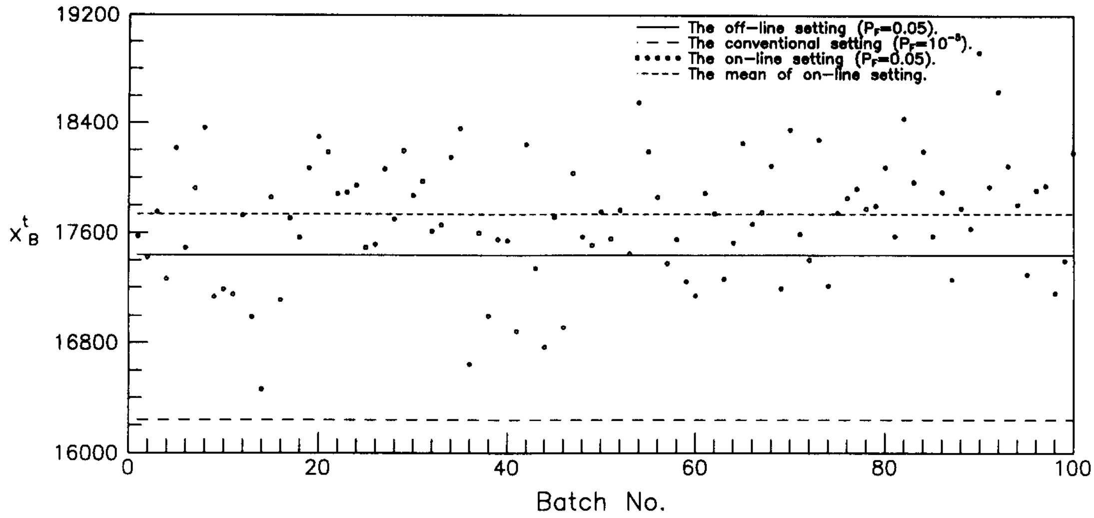

Fig. 3. The comparison between the off-line and on-line setting.

monitored with on-line sensors. There are six possible sensor sets in the present case. Also notice that the task of constructing alarm generation logic is essentially equivalent to that of determining the form of the alarm function $f(\mathbf{y})$.

Due to the limitation of space, detailed calculation are not presented here. It was found the best choice for the present example is to implement a typical two-out-of-three logic, i.e.

$$f(y_1, y_2, y_3) = (1 - y_1)y_2y_3 + y_1(1 - y_2)y_3 + y_1y_2(1 - y_3) + y_1y_2y_3 \tag{20}$$

where y_s ($s = 1, 2, 3$) is defined in Eq.(11) and the corresponding sensor set $\mathcal{M}$ is $\{(1,1), (2,2), (3,3)\}$.

CONCLUSION

Several statistical operating strategies for charging the batch reactors are presented in this paper. Based on measurement data, either off-line or on-line target setting procedure can be implemented to achieve a given level of reliability. In addition, the optimal 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.

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