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Optimal Implementation of On-Line Optimization

Xueyu Chen[1], Ralph W. Pike[1], Thomas A. Hertwig[2] and Jack R. Hopper[3]

1. Louisiana State University, Baton Rouge, LA 70803 USA, 2. IMC Agrico Company, Convent, LA 70822 USA, 3. Lamar University, Beaumont, TX 77710 USA

Abstract

Results from a theoretical and numerical evaluation of on-line optimization algorithms were used to recommend the best way to conduct on-line optimization. This optimal procedure conducts combined gross error detection and data reconciliation to detect and rectify gross errors in plant data sampled from the distributed control system. The Tjoa-Biegler method (the contaminated Gaussian distribution) was used for gross errors in the range of 3σ - 30σ or the robust method (Lorentzian distribution) for larger gross errors. This step generates a set of measurements containing only random errors which is used for simultaneous data reconciliation and parameter estimation using the least squares method. Updated parameters are used in the plant model for economic optimization that generates optimal set points for the distributed control system. Applying this procedure to a Monsanto sulfuric acid contact plant, a 3% increase in profit and a 10% reduction in SO_2 emissions were projected over current operating condition which is consistent with other reported applications.

Keywords: On-line optimization; data reconciliation parameter estimation; process optimization

Introduction

On-line optimization provides a means for maintaining a plant near its optimum operating conditions by providing set points to the plant's distributed control system. This requires the solution of three nonlinear programming problems (NLPs): for combined gross error detection and data reconciliation, for parameter estimation and for process optimization. The plant model is a set of constraint equations in the NLPs and has to match the current performance of the plant. The parameters in the plant model are updated using data sampled from the distributed control system that has been processed through gross error detection and data reconciliation procedures. The execution frequency for set point updating is based on the settling time of the process, i.e. the time required for the process to move from one set of steady-state operating condition to another.

In this paper we summarize results of a study to investigate the best way to conduct on-line optimization, and this includes a theoretical and numerical evaluation of algorithms used in on-line optimization. Previous studies have been overviews of industrial applications or focused on individual components of on-line optimization. To date, there have been no detail descriptions of the structure of on-line optimization. This work used a new sulfuric acid plant equipped with a Bailey INFI 90 distributed control system designed by Monsanto and operated by IMC Agrico. A complete description of the methodology is available (Chen, 1998) and is summarized here.

To summarize industrial applications of on-line optimization, Ayala (1997) reviewed the 31 Aspen CLRTO systems in operation and 21 in progress of which about 50% were refinery applications, 30% were ethylene plants and 20% were chemical processes. The CLRTO system included an open form process model, large-scale SQP optimizer, steady state detection, data validation and interfaces to operations personnel. Successful applications required a constrained multi-variable control system, and payouts were less than a year. Other recent industrial applications include Kelly, et al. (1996), and Bayles, (1996) that reported 3 to 15% increase in profit and improvements in plant operations.

Important recent results for gross error detection, data reconciliation and parameter estimation were reported by Albuquerque, Biegler and Kass (1997), Albuquerque and Biegler (1993), Crowe (1994); Johnston and Kramer (1995), for steady state systems and Albuquerque and Biegler (1996) for dynamic systems. Others included the measurement test method using the normal distribution (Mah and Tamhane 1982), the Tjoa-Biegler method using a contaminated Gaussian distribution (Tjoa and Biegler, 1991), and the robust function methods using the Lorentzian distribution (Huber, 1981 and Johnston and Kramer 1995) and the Fair function (Albuquerque and Biegler, 1995). Evaluations of these methods used hypothetical process models that had all measured variables.

Albuquerque and Biegler (1996) and Johnston and Kramer (1995) briefly discussed the theoretical evaluation of algorithms using the influence function. Serth and Heenan (1987) have compared the performance of the modified iterative measurement test (MIMT) and related algorithms and concluded that MIMT represents the best combination of computation speed and efficiency (accuracy). Kim, et al., (1997) reported that performance of MIMT was enhanced by a using nonlinear program (NLP) technique for a simple adiabatic CSTR process that has six variables and three constraints.

Summarizing the status of the steps in on-line optimization, gross errors can be detected by time-series

screening and statistical methods. The screening method removes values that are not within the bounds set for the process variable, and this procedure is incorporated in current industrial systems. However, screening methods can not detect persistent gross errors such as instrument bias and process leaks. Statistical methods can detect these errors, but they are more complicated and require a detailed plant model. They provide the most effective way to detect the gross errors in plant data.

Least squares or measurement test is the only statistical method that has been reported which has been applied to actual chemical and refinery processes (Simulation Science, 1991). The normal distribution used by this method can cause biased estimates for reconciled variables when gross errors are present. Therefore, methods for gross error detection have been proposed using the contaminated Gaussian distribution and robust functions that are relatively insensitive to the presence of gross errors.

Errors-in-variables models are required for parameter estimation since all measured variables in chemical plants contain random errors and possibly gross errors (Kim, Liebman and Edgar, 1990). Least squares, likelihood function, and Bayesian methods have been used for traditional parameter estimation (Stewart, Caracotsios and Sorensen, 1992), and they can be modified for use in on-line optimization. The optimization problem from parameter estimation is difficult to solve since the optimal values are usually in the interior of the region and not constrained on the boundary, Ayala (1997).

Economic optimization in on-line optimization generates a set of optimal set points for the plant that maximizes profit. Also, the optimization objective can include minimizing waste generation and energy consumption or maximizing product quality.

Mathematical programming languages such as GAMS and AMPL make formulation straightforward. Also they provide several efficient solvers, eg., MINOS and CONOPT (Chen, et al, 1996).

A precise plant model is necessary to simulate the process for on-line optimization. It serves as constraints for data reconciliation, parameter estimation and economic optimization. For industrial processes an open form equation based model is required, Ayala (1997). Closed form sequential modular models do not have the computation speed and solution robustness.

The sulfuric acid contact process at IMC Agrico Company's plant in Convent, Louisiana was used for evaluating methods for the best way to conduct on-line optimization. Also, an interactive on-line optimization program has been developed which can be used to apply these methods to a new installation. The following paragraphs describe these methods and their use in the on-line optimization program.

Methods for On-Line Optimization

In on-line optimization three nonlinear programs are solved for combined gross error detection and data reconciliation, simultaneous data reconciliation and parameter estimation, and plant economic optimization. Each optimization problem has a similar mathematical statement.

Optimize:	**Objective function**	(1)
Subject to:	**Constraints from plant model**	

The objective function is a joint distribution function for data reconciliation or parameter estimation and a profit function (economic model) for plant economic optimization. The constraint equations include material and energy balances, chemical reaction rates, thermodynamic equilibrium relations, among others.

There are two ways to conduct on-line optimization. One is the traditional way that has three nonlinear optimization problems solved sequentially (two step method). In simultaneous gross error detection and data reconciliation, gross errors in the plant data are eliminated or rectified, and we propose that a set of measurements with only random errors be constructed by using rectified values for variables with gross errors. This provides measurements with only random errors for simultaneous data reconciliation and parameter estimation. Then updated values of parameters are used in the plant model for economic optimization to generate the optimal set points for plant DCS. In the other way, we propose that gross error detection, data reconciliation, and parameter estimation be conducted simultaneously to rectify gross errors, reconcile process variables, and estimate plant parameters by solving one nonlinear programming problem (one step method). Then, economic optimization is conducted to determine the optimal set points. A comparison of these two methods is given in the Results and Discussion section.

Algorithms for Combined Gross Error Detection and Data Reconciliation

The process data from a distributed control system is subject to random and gross error, and the gross error must be detected and rectified before the data is used to estimate plant parameters. Simultaneous gross error detection and data reconciliation algorithms are used to detect and rectify the gross errors in measurements. These algorithms are measurement test method using a normal distribution, Tjoa-Biegler's method using a contaminated Gaussian distribution, and robust method using robust distribution functions.

Measurement Test: The measurement test method assumes all measurements are subject to only random errors with known normal distributions under null hypothesis and the measurement errors are independent of each other. The measurement errors are estimated by maximizing the joint probability density function or minimizing the sum squares of the standardized measurement errors, $\mathbf{e^T S^{-1} e}$, subject to constraints which are the process model. This is the well-known least squares method, and it is expressed as:

$$\underset{\mathbf{x},\,\mathbf{z}}{\textit{Minimize}}: \quad \mathbf{e}^{\mathbf{T}}\mathbf{S}^{-1}\mathbf{e} = (\mathbf{y}-\mathbf{x})^{\mathrm{T}}\mathbf{S}^{-1}(\mathbf{y}-\mathbf{x}) \qquad (2)$$

$$\textit{Subject to}: \quad \mathbf{f}(\mathbf{x}, \mathbf{z}, \mathbf{q}) = 0$$
$$\mathbf{x}^{\mathbf{L}} \le \mathbf{x} \le \mathbf{x}^{\mathbf{U}}, \; \mathbf{z}^{\mathbf{L}} \le \mathbf{z} \le \mathbf{z}^{\mathbf{U}}.$$

where equality constraints **f**, are functions of measured variables **x,** unmeasured variables **z** and parameters **q**, **y** are the measurements sampled from distributed control system. In addition, there are upper and lower bounds on the process variables. The relation between measurements **y** and the true values **x** for measured variables is defined by **y** = **x** + **e** where the vectors **e** represents the measurement errors that could be random or gross errors. Also, **S** is the diagonal matrix of the known variances σ_i^2 of measurement errors **e**.

Solving Eq. 2 will estimate the true values for the measured variables **x** and unmeasured variables **z**. Then, the measurement errors can be determined by **e = y - x**. In Eq. 2, **q** is a constant vector representing the plant parameters.

After data reconciliation, the measurement errors are determined. Then each measurement error is examined to see if it contains a gross error using a test statistic. See Chen (1998) and Mah (1990) for details. If the value of test statistic, $|e_i|/\sigma_i$, exceeds a critical value C, then this measurement is said to have a gross error. Otherwise, it contains only random error.

Tjao-Biegler Method: Tjoa and Biegler (1991) and Albuquerque and Biegler (1995) have proposed a contaminated Gaussian distribution function to describe the measurement errors. A measurement is subject to either random or gross error. The two possible outcomes are: G = {Gross error occurred} with prior probability η and R = {Random error occurred} with prior probability $(1-\eta)$. Therefore, the distribution of a measurement error is: $P(y_i \mid x_i) = (1-\eta)P(y_i \mid x_i, R) + \eta\, P(y_i \mid x_i, G)$ where $P(y_i \mid x_i, R)$ is the probability distribution of a random error and $P(y_i \mid x_i, G)$ is the probability distribution of a gross error.

It was assumed that the random errors are normally distributed with a zero mean and a known variance σ_i^2. Also, it was assumed that the gross errors are subject to a contaminated normal distribution which has a zero mean and larger variance $(b\sigma_i)^2$, $(b >> 1)$. If the measurement errors are independent of each other, then the likelihood function (or joint probability function) for all measurements are the products of the distributions for individual measurement, and the measurement errors are estimated by minimizing the negative logarithm of the joint probability density function. This gives the objective function used with the constraints of Eq. 2 for Tjoa-Biegler's method as:

After data reconciliation, each measurement is examined with a test statistic to see if it contains a gross error. See Chen (1998) and Tjoa and Biegler (1991) for details.

The basic idea of robust estimation is to build a robust distribution function ρ that is asymptotic to the normal distribution or any pre-assumed rigorous distribution function that describes the distribution pattern of measurement errors under some ideal assumptions. The estimator (mean or variance) determined by the robust distribution is insensitive to extreme observations and yet maintains a high efficiency (lower dispersion).

Robust Method: Two robust functions have been proposed in literature for mean estimation, and they are applicable for rectifying gross errors in data sampled from the DCS. These robust functions are the Lorentzian distribution proposed by Johnston and Kramer (1995), that was originally presented by Huber (1981), and the Fair function proposed by Albuquerque and Biegler (1995).

Lorentzian distribution function for a measurement error is given as:

$$r(e_i) = \frac{1}{1 + \frac{1}{2}e_i^{\,2}} \qquad (4)$$

where ε_i is the standardized measurement error, i.e., $\varepsilon_i = e_i/\sigma_i = (y_i - x_i)/\sigma_i$.

The robust function of measurement error using Lorentzian distribution is the sum of the individual distribution, and the objective function for the robust method with Lorentzian distribution used with the constraints of Eq. 2 is:

$$\underset{\mathbf{x},\,\mathbf{z}}{\text{Maximize:}} \quad r(e) = \sum_i \frac{1}{1 + \frac{1}{2}e_i^{\,2}} \qquad (5)$$

The Fair distribution function for measurement error is given as:

$$r(e_i) = c^2\left[\frac{|e_i|}{c} - \log\left(1 + \frac{|e_i|}{c}\right)\right] \qquad (6)$$

The objective function for the robust method with Fair function (Albuquerque and Biegler, 1995) used with the constraints of Eq. 2 is:

$$\underset{\mathbf{x},\,\mathbf{z}}{\textit{Minimize}}: \quad -\sum_i \left\{\ln\left[(1-h)e^{\frac{-(y_i - x_i)^2}{2s_i^2}} + \frac{h}{b}e^{\frac{-(y_i - x_i)^2}{2b^2 s_i^2}}\right] - \ln\left[\sqrt{2p}\, s_i\right]\right\} \quad (3)$$

$$\underset{\mathbf{x,\ z}}{Minimize}: r(e) = \sum_i c^2 \left[\frac{|e_i|}{c} - \log\left(1 + \frac{|e_i|}{c}\right) \right] \quad (7)$$

where c is a tuning parameter. The Fair function is convex and has continuous first and second derivatives (Albuquerque and Biegler, 1995).

Evaluation of Distributions Functions for Data Reconciliation and Gross Error Detection

The theoretical evaluation of the algorithms is based on the robustness and precision of an estimator from a distribution function (Seber, 1984). Robustness of an algorithm is the ability to ignore the contribution of extreme data, i.e., insensitive to the presence of gross error; and it is measured by the influence function of the distribution function. The precision of an estimator is given by the accuracy of the estimated value, and it is measured by the relative efficiency of a distribution function. The relative efficiency is defined as the ratio of the variances obtained from two distribution functions (Larsen and Marx, 1986).

The influence function quantifies the influence of a measurement on the estimated value in data reconciliation. For M-estimate, the influence function is proportional to the derivative of a distribution function with respect to the measured variable, ($\partial\rho/\partial x$) (Huber, 1981 and Hampel, et al., 1986), i.e.,

$$IF \propto \partial\rho/\partial x \quad (8)$$

For the normal distribution used in the measurement test method it can be shown, Chen (1997), that the influence function is:

$$IF_{MT} \propto \frac{\partial r}{\partial x_i} = \frac{y_i - x_i}{s_i^2} = \frac{e_i}{s_i} \quad (9)$$

As shown in Eq. 9, the influence function is proportional to the standardized measurement error, $\epsilon_i = (y_i - x_i)/\sigma_i$, and it is not bounded when the measurement error becomes infinite as shown in Figure 1. This means that the least squares method is unable to bound the effect of large gross errors on the estimation of reconciled measurements. The presence of gross errors will result in biased estimation of reconciled measurements from measurement test, and the degree of bias is proportional to the magnitude of the gross errors.

For the contaminated Gaussian distribution used in the Tjao Biegler's method, it can be shown, Chen (1998), that the influence function is:

$$IF \propto \frac{\partial r}{\partial x^i} = \frac{\frac{(y^i - x^i)}{s^i}\left\{(1-h)e^{\frac{-(y_i-x_i)^2}{2s_i^2}\left(1-\frac{1}{b^2}\right)} + \frac{h}{b^3}\right\}}{(1-h)e^{\frac{-(y_i-x_i)^2}{2s_i^2}\left(1-\frac{1}{b^2}\right)} + \frac{h}{\cdot}} = \frac{\frac{e^i}{s^i}\left\{(1-h)e^{\frac{e_i^2}{2}\left(1-\frac{1}{b^2}\right)} + \frac{h}{b^3}\right\}}{(1-h)e^{\frac{e_i^2}{2}\left(1-\frac{1}{b^2}\right)} + \frac{h}{\cdot}} \quad (10)$$

As shown in Eq. 10, the influence function for the contaminated Gaussian distribution is a function of the standardized measurement error, $\epsilon_i = (y_i - x_i)/\sigma_i$. For small errors e.g., $\epsilon_i < 2$, the exponential term in the Eq. 10 is much larger than the second term η/b^3 (or η/b) for $\eta = 0.5$ and $b = 10$. For this case the influence function simplifies to the equation obtained for normal distribution, Eq 9; and it is the same as one for the measurement test method. The contaminated Gaussian distribution acts like a normal distribution for small errors as shown in Figure 1. The distribution function for random error dominates the contaminated Gaussian distribution, and the distribution for the gross error does not contribute.

For larger errors, e.g., $\epsilon_i > 4$, the exponential term in Eq. 10 is much smaller than the second term η/b^3 (or η/b) for $\eta = 0.5$ and $b = 10$. The influence function can be simplified to give:

$$IF \propto \frac{y_i - x_i}{(b s_i)^2} = \frac{1}{b^2}\frac{e_i}{s_i} \quad (11)$$

For larger errors, the distribution function for gross errors dominates the contaminated Gaussian distribution. As shown in Eq. 11, the influence function of the contaminated distribution function is the same as the normal distribution but with the magnitude reduced by b^2. This influence function is still a function of the error

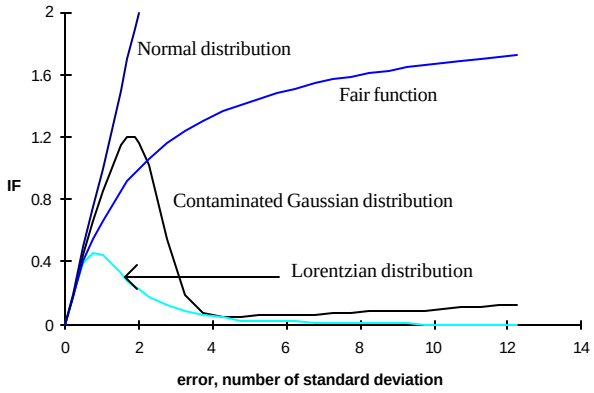

Figure 1 Influence Functions of Distributions

magnitude as shown in Figure 1, and it is unbounded when the error becomes infinite.

In the contaminated Gaussian distribution, b is a tuning parameter to shape the distribution. Increasing b will reduce the effect of a gross error on the estimation and increase the robustness of this approach. However, it will decrease the asymptotic efficiency to the normal distribution. In the practical applications, b is usually chosen between 10-20; and therefore the effect of a gross error on the estimation is reduced 100-400 times compared with the measurement test method. Also, gross errors are rarely infinite, and generally they are of moderate magnitude (about 5σ to 20σ). Hence, for gross

errors of this magnitude the effect of gross errors on data reconciliation is negligible using the contaminated Gaussian distribution. Therefore, it is concluded that a method based on the contaminated Gaussian distribution should be robust for the estimation of reconciled measurements when gross errors are of a moderate magnitude.

The Lorentzian distribution function was given by Eq. 4, and its influence function is:

$$\mathrm{IF}_{\mathrm{Lorentzian}} \propto \frac{\partial r}{\partial x_i} = -\frac{e_i}{\left(1+\frac{1}{2}e_i^2\right)^2} \qquad (12)$$

As shown in Figure 1, the influence function of Lorentzian distribution depends on the error size, and IF increases and then decreases with increasing error. The IF of the Lorentzian distribution has the advantage that it has larger values for measurements with smaller (random) errors and has smaller values for measurements with larger (gross) errors. This means that a method based on the Lorentzian distribution should not be affected by contributions from measurements with gross errors.

The Fair function is given in Eq. 7, and its influence function is:

$$\mathrm{IF}_{\mathrm{Fair}} \propto \frac{\partial r}{\partial e_i} = c^2\left(\frac{1}{c}-\frac{\frac{1}{c}}{1+\frac{|e_i|}{c}}\right) = \frac{1}{\frac{1}{|e_i|}+\frac{1}{c}} \qquad (13)$$

As shown in Figure 1, this influence function increases with increasing error and approaches a constant c. The effect of gross errors on a method based on this distribution is bounded by the value c when the error becomes infinite. The parameter c in Fair function determines the robustness and efficiency of the estimation. Smaller values of c will give a more robust method, but it will be less efficient. A method based on the Fair function is able to bound the effects of very large gross errors.

A effective distribution function for a data reconciliation algorithm has to be insensitive to the presence of gross error and efficient for measurements with random errors. The influence functions for four distributions are essentially the same for errors up to 1σ. The influence function of Lorentzian distribution function is the least sensitive of the four to errors as shown in Figure 1. The influence function for the normal distribution increases linearly with the increasing errors, and biased estimates are obtained if measurements with large gross errors are used in data reconciliation. The influence function for the Fair function is similar to the normal distribution, except that it is bounded for larger (gross) errors. Compared with the normal distribution, it is less sensitive to the presence of larger gross errors and is able to bound the effect of extremely large gross errors. However, it gives biased estimation when measurements with large gross errors are included in the data for data reconciliation. The influence function for contaminated Gaussian distribution increases with increasing errors to 2σ, decreases to 4σ, and then increases linearly at a much lower rate. It is relatively insensitive to errors, but it has the unbounded nature of the normal distribution for errors larger than 50σ.

In summary, the evaluation of influence functions for the probability distributions shows that the contaminated Gaussian and Lorentzian distributions have influence functions that are relatively insensitive to gross errors. Methods based on the contaminated Gaussian distribution should have the best performance for reconciling measurements when moderate size gross errors are present; and methods using the Lorentzian distribution should be more effective for very large gross errors.

Process Description

The IMC Agrico contact plant in Convent, Louisiana was designed by the Enviro-Chem System Division of Monsanto and began operation in March, 1992. It produces 3200 TPD 93 %(wt) sulfuric acid and process steam as a by-product, and it has a Bailey INFI 90 distributed control system. This process incorporates many of the types of process units found in chemical plants such as packed bed catalytic reactors, absorption towers and heat exchanger networks, among others. It represents the state-of-art contact sulfuric acid technology.

In the contact process, molten sulfur is combusted with dry air; and the reaction is exothermic and goes to completion in the sulfur furnace. The gas leaving the burner is composed of sulfur dioxide, nitrogen, and unreacted oxygen at approximately 1400^{o}K. Heat from this gas is recovered in the waste heat boiler as byproduct steam. The gas enters the packed bed catalytic reactor that consists of four beds packed with two different types of vanadium pentoxide catalyst. Here sulfur trioxide is produced from sulfur dioxide, and the reaction is exothermic and approaches equilibrium exiting each bed. Heat is removed to shift the equilibrium, and this heat is used to produce steam. Also, the equilibrium conversion is increased in the fourth catalyst bed by removing SO_3 in the inter-pass absorption tower. In the final absorption tower, SO_3 is removed from the gas with 98 wt% sulfuric acid. Gases exiting the final absorption tower go to the stack with less than 400 ppm SO_2 as required by regulations for emissions, no more than 4.0 lb of sulfur dioxide per ton of sulfuric acid produced.

Process Model

A open form model was developed from the process flow diagram and process design data. The packed bed catalytic reactor was simulated with a kinetic

model developed by Harris and Norman (1972) and Richard (1987). The process model has 43 measured variables, 732 unmeasured variables, 11 parameters and 761 linear and nonlinear equality constraints. The model equations were programmed in GAMS (General Algebraic Modeling System), and the process model was incorporated in the three optimization programs using GAMS/CONOPT. A comparison of results from the process model with the plant design data was made to assess the validity and accuracy of the simulation. The simulation matched the plant design data within the accuracy of the data. Also, a comparison was made with process data taken from the plant operating five years after start-up, and the simulation with parameters updated with reconciled plant data agreed within the accuracy of the data, e.g. outlet temperatures from the packed bed reactors agreeing within 3°F. Details of these comparisons are given by Chen (1998).

Process Measurements

The 43 process measurements obtained from the distributed control system included 25 temperature, 11 flow rate, 2 pressure and 5 composition measurements. The standard deviations were determined based on 61 plant data set from 11 consecutive days. These process variables and their associated standard deviations are given by Chen (1998). Of these 43 measurements, 18 are required to determine the state of the process

Results and Discussion

Process Optimization: Three optimization programs for on-line optimization were written in GAMS for simultaneous gross error detection and data reconciliation, simultaneous data reconciliation and parameter estimation, and plant economic optimization. The gross error detection and data reconciliation program has options to use the least squares method, the contaminated Gaussian distribution, and the Lorentzian function. The simultaneous data reconciliation and parameter estimation program uses the least squares method. Also, a plant data file from DCS and parameter file from the previous on-line optimization are included for use by the simultaneous gross error detection and data reconciliation program. This program is executed to generate a file of plant data that contains only random errors. This data file is used in simultaneous data reconciliation and parameter estimation program, and executing the parameter estimation program generates a file of estimated process parameters and a file of reconciled plant measurements. The parameter file is used in the economic optimization, and the economic optimization program generates a file containing the optimal set points to be sent to a distributed control system. In addition, comprehensive output files are generated for each optimization program.

Two sets of plant data from DCS were used to evaluate on-line optimization of the contact process, and the details of these optimal solutions are reported by Chen (1998). Six measurements of the total of 43 were detected as containing gross errors using the contaminated Gaussian function option. These were four temperatures, a flow rate and a composition, and they were caused by incorrectly calibrated instruments. These values were replaced by reconciled data, and the simultaneous data reconciliation and parameter estimation program was executed. Then the updated parameters were used in the plant model for economic optimization to obtain the optimal set points for the DCS. For the two sets of plant data, economic optimization gave an increased profit of 2.3% (or $313,000/year) and 3.1% (or $410,000/year) over current operating conditions. Also, 1.8% and 2.7% increase in profit were obtained with a 10% reduction in SO_2 emissions for the two set of plant data. This is consistent with other reported applications of on-line optimization and could lead to a typical payback of one year (Ayala, 1997).

Several other cases were reported by Chen (1998) with increased profits and reduced emmissions comparable to those above. Also, the least squares and Lorentzian function options of the combined gross error detection and data reconciliation program were used with the plant data. The least squares option only detected three of the gross errors, and the Lorentzian function option incorrectly detected eight more gross errors than the contaminated Gaussian function option. These results are consistent with the theoretical performance of these methods as discussed earlier.

An evaluation of the sensitivity of the reconciled data to the process parameters was conducted using data from the DCS, and the plant design data. An average difference of 10% in the parameters gave a comparable difference in the reconciled data.

One and Two Step Methods: The two ways to conduct on-line optimization were evaluated using 215 sets of simulated plant data. The two-step method had a 4% smaller variation on estimated parameter values, 6.5% larger error reduction, and 10.6% larger relative standard deviation reduction on reconciled data than one-step method. Also, the two step method had 6.3% larger gross error detection rate and committed 50% less of type I errors than the one-step method. The two-step method required 82% more computation time than the one-step method. In summary, both one-step and two-step were able to accurately estimate the plant parameters and process variables for the sulfuric acid process. Two-step method had better performance than the one-step method but required more computation time. Also, the one-step method eliminates the interaction between two data reconciliations for gross error detection and for parameter estimation.

Numerical Evaluation of Combined Gross Error Detection and Data Reconciliation Methods

The measurement test, Tjao-Biegler (contaminated Gaussian distribution) and robust (Lorentzian distribution) methods were evaluated using the plant design data as the true values for the measured variables. 645 sets of simulated plant data were

constructed from the plant data by adding random error and one to four gross errors with magnitudes of 3σ, 5σ, 10σ, 20σ, and 30σ randomly.

For the single gross error cases, detailed statistical results were obtained from 2560 runs. These included gross error detection rate, number of type I errors, and error reductions for these algorithms; and the details are reported by Chen (1998). It was found that the Tjoa-Biegler method has highest gross error detection rates for the gross errors ranging in 3σ to 30σ followed by the robust method. Also, the Tjoa-Biegler method had the smallest number of type I errors, highest random and gross error reduction for the gross error size from 3σ to 30σ. The robust method was superior to the Tjoa-Biegler method when a gross error was larger than 30σ which agrees the theoretical evaluations.

For the multiple gross error cases, detailed statistical results were obtained from 2560 runs, and the details are reported by Chen (1998). The comparisons showed that the Tjoa-Biegler and robust methods committed small numbers of type I errors than the others. A modified compensation strategy proposed by Chen (1998) was incorporated with measurement test method, and it was conducted with the same simulated plant data as other methods. The modified compensation measurement test (MCMT) method significantly reduced the misrectification that was committed by the measurement test method for multiple and larger gross errors.

For both single and multiple gross errors the Tjoa-Biegler method had the best performance for moderate gross error size (3σ - 30σ) in simultaneously rectifying both random and gross errors. The robust method was the best when gross errors were larger than 30σ. The measurement test method had significant biased reconciled measurements. The robust method was the least sensitive to the variations of the gross error size, and measurement test method was the most sensitive.

Summary and Conclusions

The optimal procedure for on-line optimization based on the results from this research is to conduct simultaneous gross error detection and data reconciliation to detect and rectify gross errors in plant data sampled from distributed control system using the Tjoa-Biegler method (contaminated Gaussian distribution) for gross errors in the range of 3σ - 30σ or the robust method (Lorentzian distribution) for larger gross errors. This step generates a set of measurements containing only random errors. Then, this set of measurements is used for simultaneous parameter estimation and data reconciliation using the least squares method. This step provides the updated parameter values in the plant model for economic optimization. Optimal set points are generated for the distributed control system from the economic optimization using the updated plant and economic models.

Interactive On-Line Optimization System

An interactive on-line optimization program is available from the authors that has a Windows interface for entering the information needed to conduct on-line optimization. Written in Visual Basic 5.0, the program uses this information to write and run the three GAMS optimization programs and generates the optimal set points for the distributed control system. Also, summary and detailed reports are prepared. Options include using least squares, the Tjao-Biegler and robust methods.

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