15th Triennial World Congress, Barcelona, Spain

RESULTS ANALYSIS FOR ITERATIVE FEEDBACK STEADY-STATE OPTIMIZATION

Jen-Hao Cheng and **Evanghelos Zafiriou**[1]

Department of Chemical Engineering
University of Maryland
College Park, Maryland 20742, U.S.A.

Abstract: An iterative feedback optimization methodology has been introduced as a complementary approach to conventional real-time optimization (RTO) methods to improve plant operation without requiring repetitive model updating. In this paper, the results analysis component that is an integral part of an RTO system is developed for use with iterative feedback optimization to evaluate the inherent variability of the optimization results transmitted from the plant measurements. Only optimization results that represent meaningful changes are implemented as the new setpoints, thus reducing unnecessary and profitless corrective actions. The effectiveness of the proposed results analysis method is tested on a simulated CSTR process. *Copyright ©2002 IFAC*

Keywords: Results analysis, Real-time optimization, Steady-state optimization, Measurement noise, Statistical process control

1. INTRODUCTION

During the operation of a chemical plant, the results of the higher level repetitive on-line optimization are used to improve process operations by determining the setpoints for the lower level feedback control systems. Results analysis evaluates the optimization results (calculated setpoints) before they are implemented in the plant via the control system, because the calculated optimization variables are subject to inherent variability caused by the variability in the plant data and transmitted through the optimization system components (Miletic and Marlin, 1998; Forbes and Marlin, 1996). The results analysis is used to distinguish the common cause variability due to measurement noise from the special cause variability caused by significant disturbances. Only optimization results that represent meaningful changes are implemented. Miletic and Marlin (1998) proposed an on-line results analysis method in real-time optimization (RTO) through the application of two fundamental techniques: sensitivity analysis and statistical process/quality control. In this paper, a statistical method based on a similar approach is proposed for on-line results analysis of the iterative feedback optimization methodology presented by Cheng and Zafiriou (2000). This is a complementary optimization approach to conventional RTO. It is based on an analogy between steady-state operation periods in process operation and iterations in numerical optimization. The process measurements are utilized to correct the gradient information directly without requiring model parameter updating.

The application of sensitivity analysis in evaluating a conventional RTO system has been addressed by Koninckx (1988) and Forbes and Marlin (1996). The common cause variability of the

[1] Author to whom correspondence should be addressed. E-Mail: zafiriou@eng.umd.edu. Tel: (301)405-6625. Fax: (301)314-9126

calculated independent variables (inputs) can be characterized by a covariance matrix and it can be calculated through sensitivity analysis (linear approximation) of the RTO system. Thus, the estimation of the covariance matrix involves two sensitivity matrices that represent the linear transformations of the plant variability through two RTO components (parameter updater and economic optimizer). In the case of the iterative feedback optimization approach (Cheng and Zafiriou, 2000), which does not require model updating, the covariance matrix estimation only involves a single sensitivity matrix which is evaluated locally at each optimization period with the model derivatives. MacGregor and Kourti (1995) applied a hypothesis test to evaluate the multivariate deviation for multivariate process or quality control. This multivariate statistical process/quality control method is used to judge whether the iterative feedback optimization has produced newly calculated input values that are significantly different from the currently implemented input policy. The goal of the on-line results analysis is to decrease the frequency of unnecessary setpoint changes and increase the operating profit.

2. METHODOLOGY

2.1 Iterative Feedback Optimization

The iterative feedback optimization methodology was designed to not require repetitive model updating by directly utilizing plant measurements to improve plant operation. This methodology is developed based on an analogy between iterations in numerical optimization and steady-state periods in plant operation as described in Table 1. The numerical optimization method used in the analogy (left column) may be any search direction algorithm that utilizes a gradient to compute a search direction and perform a line search along the direction. The plant operation is an integral part of the optimization, as shown on the right column, with each iterate during the line search therefore representing a steady-state operation period. To maximize the profit when utilizing a minimization standard, the objective function, Φ, can be defined as the negative of the profit. The goal is to compute and maintain the optimal operating policy, consisting of the inputs u, which have economic impact on the plant operation directly and through the plant outputs they affect. Although the gradient equations are constructed based on the model, the model error can be compensated for by explicitly incorporating the measured plant outputs (y), instead of the model predictions ($\tilde{y}$), to update the approximate gradient for the objective function (g_{app}). It is noted that if constraints

Table 1. Iterative feedback optimization.

Numerical Optimization	**Plant Operation**
$\min_u \Phi(u, y)$	$\min_u \Phi(u, y)$
$u_l \leq u \leq u_u$	$u_l \leq u \leq u_u$
	$\lvert u_i - u_{i-1} \rvert \leq \Delta u_{max}$
and	and
$\tilde{F}(u, y) = 0$ (model)	$F(u, y) = 0$ (plant)
<u>i^{st} iteration</u>	<u>i^{st} s.s. period</u>
1. Solve the model	**1. Operate the plant**
$u_i \rightarrow Model \rightarrow \tilde{y}_i$	$u_i \rightarrow Plant \rightarrow y_i$
(Model predictions)	(Plant measurements)
2. Compute gradient	**2. Compute gradient**
$\tilde{g}(u_i, \tilde{y}_i)$	$g_{app}(u_i, y_i)$
3. Search direction	**3. Search direction**
$\tilde{g} \rightarrow Algorithm \rightarrow d$	$g_{app} \rightarrow Algorithm \rightarrow d$
4. Line search	**4. Line search (n_s tries)**
$u_{i+1} = u_i + \alpha d$	$u_{i+1} = u_i + \alpha d$
$\alpha_1 = 1$ ($1st$ trial value)	$\alpha_1 = 1$ ($1st$ trial value)

exist then the corresponding gradients should be provided too.

For optimizing an existing process, two tuning parameters should be provided by the users: Δu_{max} is used to specify the maximum allowed policy changes between successive steady-state periods during operation to prevent aggressive changes that may not be acceptable from a practical point of view; n_s is used to specify the maximum number of a line search to save operation cost by avoiding meaningless corrective actions that may only result in extremely small improvement. To further compensate for model error that may on occasion be too large, recomputing of the search direction is introduced if an improvement direction cannot be found after n_s tries in a line search. Resetting the Hessian to identity ($H = I$) is first performed to compute a new direction and, if necessary, this newly computed direction is reversed to seek further improvement opportunity. The details of the approach can be found in Cheng and Zafiriou (2000). Therefore, iterative feedback optimization pursues the rather conservative goal of improving operation gradually and this enhances its robustness with respect to significant structural model error with which conventional RTO may not be able to deal by parameter updating only. In this paper, the on-line statistical results analysis method used in RTO is extended to iterative feedback optimization with the necessary modifications.

2.2 Variability Transformation

Statistical results analysis techniques depend on an estimation of the common cause variability of the calculated independent optimization variables (setpoints). The results analysis component is introduced into an optimization system to check the variability of independent variables. Thus the system is made "open-loop" first by results analysis to evaluate the optimization results and is back to closed-loop mode if the change between calculated values and current values is significant (special cause variability). Figure 1 illustrates the open-loop optimization system where ν represents the high frequency noise (common cause variability). The feedback optimizer incorporates the current input policy, u_i, and the current plant measurements, y_i, to compute the new input policy u_{i+1} through evaluating the objective function, Φ, the model equations, $\tilde{F}$, and the gradient information, g. The lower frequency and nonstationary disturbances (special cause variability), which really affect the operation significantly, can be reflected in the model-plant mismatch (F represents the true plant equation).

The variability in the calculated independent optimization variables can be characterized by a covariance matrix Q. This can be approximately computed with the linear approximation of the open-loop optimization system which conveys the variability of plant measurement through the feedback optimization component. Thus, the open-loop approximation of Q can be computed by applying a linear transformations to the estimated covariance matrix of the plant measurements U. This covariance matrix U describes only the common cause variability arising from measurement noise (high-frequency disturbances) and can be obtained by collecting plant data between optimization periods and by estimating the covariance matrix with statistical methods. As a result, the covariance matrix Q can be evaluated by multiplying U by the sensitivity matrix of the feedback optimizer (du/dy):

$$Q = \left(\frac{du}{dy}\right) U \left(\frac{du}{dy}\right)^T \tag{1}$$

For computational convenience, the inverse matrix of Q is calculated instead:

$$Q^{-1} = \left(\frac{dy}{du}\right)^T U^{-1} \left(\frac{dy}{du}\right) \tag{2}$$

where the sensitivity matrix (dy/du) describes the differential change in the plant measurements in response to a differential change in the inputs. It can be calculated in light of the reduced gradient method (Edgar and Himmelblau, 1988), which is used to construct gradient equations used by iterative feedback optimization for algebraic equation models:

$$\frac{dy}{du} = -\left(\frac{\partial \tilde{F}}{\partial y}\right)^{-1} \left(\frac{\partial \tilde{F}}{\partial u}\right) \tag{3}$$

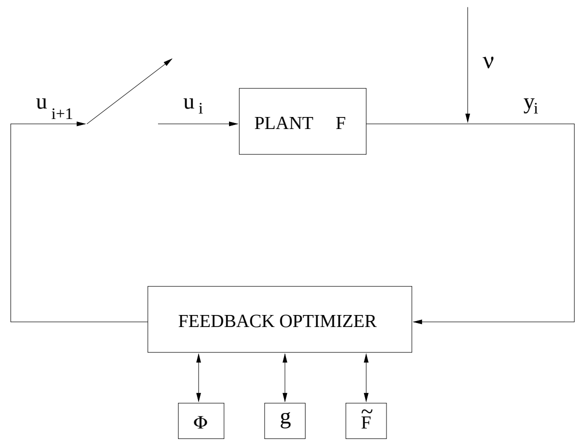

Fig. 1. Open-loop optimization system.

The model derivatives are evaluated locally at each iteration with plant measurements and corresponding inputs.

2.3 Hypothesis Test

Statistical process or quality control (SPC/SQC) is a fundamental approach to results analysis to determine if the calculated optimization results represent meaningful change in plant operation (Miletic and Marlin, 1998). MacGregor and Kourti (1995) applied a hypothesis test based on the Hotelling T^2 statistic to the multivariate statistical process or quality control methods which take into account the interactions among process variables. Miletic and Marlin (1998) have successfully implemented these SPC/SQC methods online to the RTO system. In this paper, a similar approach is applied to the iterative feedback optimization system to evaluate the calculated input policy. First, the multivariate deviation between the currently applied input policy (u_i) and the calculated input policy (u_{i+1}) is estimated by the Hotelling T^2 statistic:

$$T^2 = (u_{i+1} - u_i)^T Q^{-1} (u_{i+1} - u_i) \tag{4}$$

The hypothesis test is stated as follows:

$$\begin{cases} H_0 : u_{i+1} = u_i \\ H_1 : u_{i+1} \neq u_i \end{cases} \tag{5}$$

By evaluating the test (5), one can determine if the calculated input policy is statistically the same as the current input policy at a specified significance level. The null hypothesis, H_0, assumes that the calculated input policy is the same as the current input policy. On the other hand, the alternative hypothesis, H_1 assumes that the calculated input policy is different from the current input policy. The upper control limit (UCL) for the hypothesis test (5) can be set to be:

$$\text{UCL} = \frac{m(N+1)(N-1)}{N(N-m)} F_\alpha(m, N-m) \tag{6}$$

where N is the number of data points collected for estimating U at each period, m is the row dimension of u, and F_α is the tabulated F statistic at significance level α with m and $N-m$ degrees of freedom. (Miletic and Marlin, 1998)

The hypothesis test (5) can be evaluated by comparing the T^2 statistic (4) to the control limit value (6). If the statistical multivariate deviation is larger than the control limit value, the test is triggered (H_0 is rejected in favor of H_1) and calculated input policy is applied to the plant. Otherwise, the input policy is not altered (H_0 is accepted) and the operating conditions of the plant remain the same. The hypothesis test is evaluated at every optimization iteration to distinguish the common cause variability and the special cause variability. However, it is not necessary to estimate the covariance matrix Q at each iteration until the process change is significant (special cause variability).

3. ILLUSTRATION

The effectiveness of the proposed results analysis method is demonstrated through a simulated case study on a typical CSTR process, which was originally studied by Zhang and Roberts (1991) for on-line steady-state optimization. A single reversible reaction is considered to be taking place in the CSTR as:

$$A + 2B \underset{k^-}{\overset{k^+}{\rightleftharpoons}} 2E + P \tag{7}$$

where

$$\begin{aligned} k^+ &= \beta_1^+ \mathrm{e}^{-\beta_2^+/T_R+273.15} \\ k^- &= \beta_1^- \mathrm{e}^{-\beta_2^-/T_R+273.15} \end{aligned} \tag{8}$$

The reactants A and B are raw materials and E and P are the reaction products. There are two input streams of mass flow rates F_A (kg/s) and F_B (kg/s) containing pure raw materials A and B, respectively, and one product stream of mass flow rate $F_A + F_B$ (kg/s) containing all four components with mass fractions of X_A, X_B, X_E and X_P. T_R (°C) is the reaction temperature and β_1^+ (s^{-1}), β_2^+ (K), β_1^- (s^{-1}) and β_2^- (K) are the reaction rate parameters. Following Zhang and Roberts (1991), several assumptions and definitions are made: (1) The inlet flow of reactant A, F_A, is fixed at 0.88 kg/s. (2) The reactor capacity (V) is fixed at 2104.7 kg. (3) The inlet flow of reactant B, F_B (kg/s), and the reactor temperature, T_R (°C), are considered as the independent optimization variables (operating policy), i.e., u=[F_B T_R]. (4) All component concentrations are the corresponding dependent

Table 2. Plant and model parameters.

Parameter	Plant	Model
β_1^+ $(1/s)$	0.61×10^{24}	0.5×10^{24}
β_2^+ (K)	21600	21800
β_1^- $(1/s)$	2.55×10^{31}	1.9×10^{31}
β_2^- (K)	27000	27200

variables (outputs), i.e., $y = [X_A \; X_B \; X_E \; X_P]$. (5) Model error is introduced in the reaction rate parameters, as listed in Table 2, to emulate model-plant mismatch. (6) The instantaneous profit to be maximized is based on the difference between the sales of products E and P and the costs of raw materials A and B:

$$\begin{aligned} \text{Profit} = &(F_A + F_B)(66.0X_P + 1.5X_E) \\ &- (4.4F_A + 6.6F_B) \end{aligned} \tag{9}$$

The performance of the iterative feedback optimization system without results analysis is simulated first on this case study. The initial input is u_1 = [1.0 85] and the optimization parameters are selected as n_s = 4 and Δu_{max}=[0.1 1.0]. Measurement noise under Gaussian distribution is introduced into the outputs with 1.2% magnitude. Figures 2 and 3 show the profit and input profiles, respectively. The solid line represents the true value and the dotted line the optimal value. In Fig. 2, the dashed line represents the measured profit value which is evaluated with process measurements rather than true inputs and outputs. The profit contours for the true process and the corresponding feedback optimization trajectory in the input space are illustrated in Fig. 4, with the true optimum indicated by an $\times$ at the center. Each optimization iteration (steady-state period) is marked by a small circle ($\circ$) along the trajectory. These results show that the robust iterative feedback optimization can compensate for the model-plant mismatch iteratively towards the true optimum within the first 22 periods, where the disturbances or process changes (contributing to model-plant mismatch) dominate the measurement noise. But the computed input variables keep fluctuating around the true optimum in the remaining periods, where the measurement noise dominates the disturbances, until the optimization is stopped when further improvement is not possible with direction reversing. A pair of resetting and reversing actions are triggered to determine an improvement direction after the regular computation is performed, resulting in the cross-shaped paths left of the true optimum in Fig. 4. The fluctuation in the input profile after the 22nd period represents unnecessary corrective actions which can cause profit loss in the true profile. Note that the noise can result in a much more

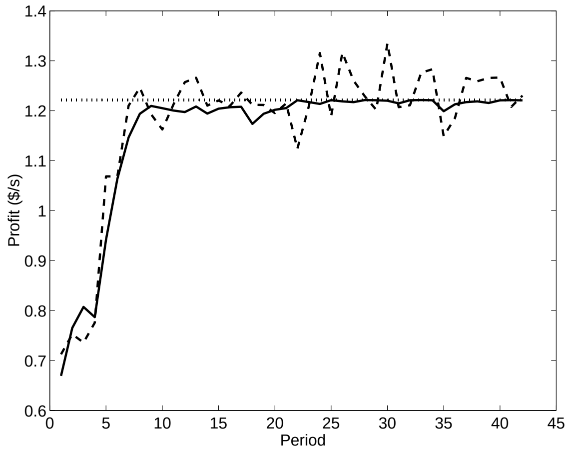

Fig. 2. Profit profile without results analysis. Solid line: true value. Dashed line: measured value. Dotted line: optimal value.

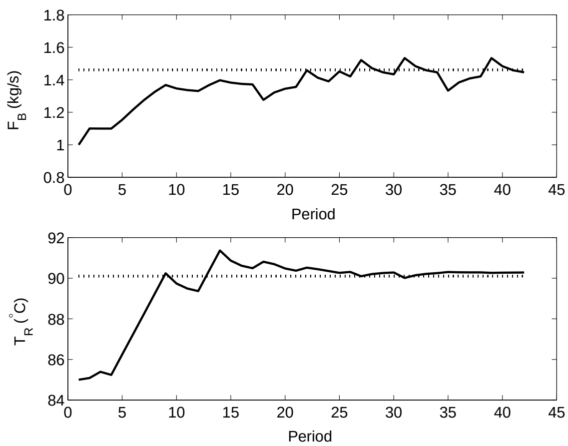

Fig. 3. Input profile without results analysis. Solid line: true value. Dotted line: optimal value.

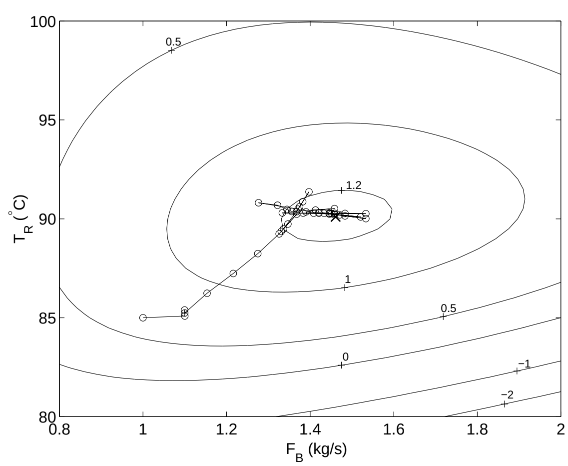

Fig. 4. Profit contours and feedback optimization trajectory without results analysis.

significant fluctuation in the measured profit than in the true profit. Although the true profit loss is not significant in this case due to the profit formulation, the unnecessary corrective actions themselves may cause extra operating costs.

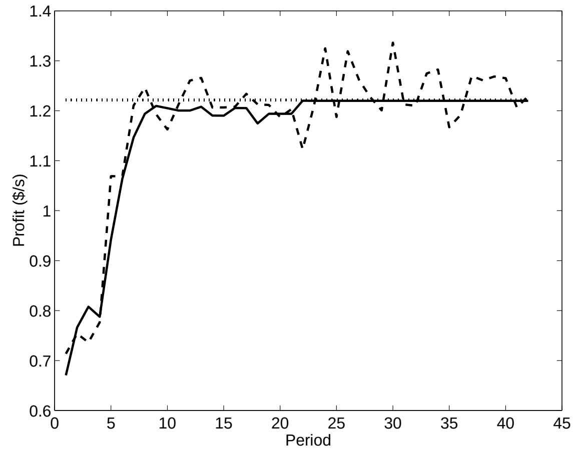

Fig. 5. Profit profile with results analysis. Solid line: true value. Dashed line: measured value. Dotted line: optimal value.

The proposed results analysis method is tested on this case study with $m = 2$ and $N = 50$ at 99% level of significance ($\alpha = 0.99$). Thus, the corresponding F statistic is $F_{0.99}(2, 48) = 5.06$ and the control limit (6) for the optimization variables (setpoints) is $UCL = 10.53$. At each steady-state period, the covariance matrix U is estimated by using 50 plant data points and the covariance matrix Q for the optimization variables is also obtained through variability analysis. Then the newly computed optimization results are analyzed by comparing the T^2 statistic to the UCL value to check if the new inputs make significant changes or not. Figures 5 - 7 illustrate the simulations with results analysis, corresponding to the simulations in Figs. 2 - 4 without results analysis, respectively. These results show that the proposed method can successfully distinguish the common cause variability (due to measurement noise) from the special cause disturbances. During the first 22 special cause periods, the computed input variables are implemented on the process to improve the operation since they are evaluated as significant changes by results analysis. On the contrary, the computed input variables are not implemented on the process in the remaining periods where the special cause signals are not triggered by the method. Thus the proposed method can successfully reduce the unnecessary corrective actions and increase the operating profit. A special cause signal is missed (H_0 is wrongly accepted) at the 14th period where the process is indeed subject to small disturbance domination (model-plant mismatch is not completely compensated for), but it does not affect the performance of the method.

4. CONCLUSION

A statistical method is proposed in this paper for on-line results analysis of iterative feedback

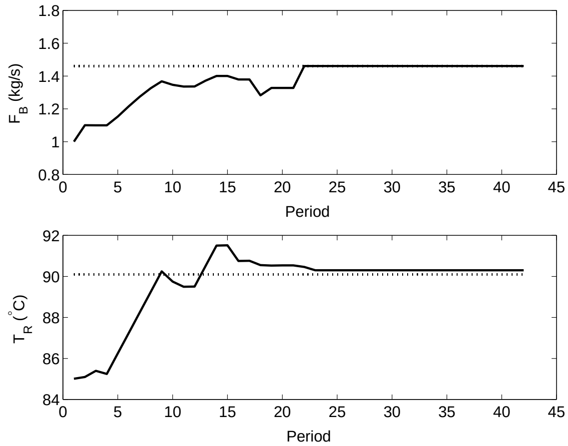

Fig. 6. Input profile with results analysis. Solid line: true value. Dotted line: optimal value.

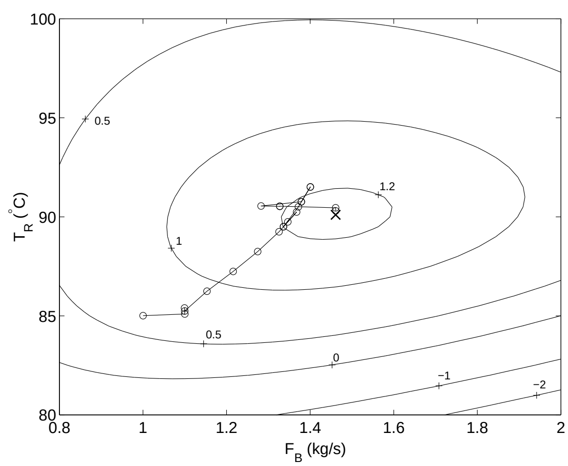

Fig. 7. Profit contours and feedback optimization trajectory with results analysis.

optimization before the optimization results (setpoints) are transmitted to the plant via the process control system. This approach is based on an extension of the RTO results analysis method which involves sensitivity analysis and multivariate statistical process/quality control. Results analysis evaluates the variability of the calculated independent variables and determine whether the variability is common cause or special cause. Only the optimization results that represent meaningful change (special cause variability) are implemented. The effectiveness of the method is tested on a CSTR process which is optimized by iterative feedback optimization. Both model-plant mismatch and measurement noise are introduced into the optimization system in simulations. The model-plant mismatch can be viewed as the result of the external disturbances (or process changes). The simulation results show that the proposed result analysis method can successfully distinguish the special cause variability from the common cause variability of the computed inputs for almost all optimization periods. During the periods where the operating conditions are far from the true optimum, the special cause signals are triggered and the optimization results are implemented in the plant to further correct for the effect of model-plant mismatch. When the operating conditions approach the optimal values, the common cause variability is detected immediately and the operating conditions remain the same. Therefore, the method allows iterative feedback optimization to effectively improve the process operation and also avoids unnecessary and profitless corrective actions.

REFERENCES

Cheng, J.-H. and E. Zafiriou (2000). Robust model-based iterative feedback optimization of steady-state plant operations. *Ind. Eng. Chem. Res.* **39**(11), pp. 4215–4227.

Edgar, T. F. and D. M. Himmelblau (1988). *Optimization of Chemical Processes.* McGraw-Hill. New York.

Forbes, J. F. and T. E. Marlin (1996). Design cost: A systematic approach to technology selection for model-based real-time optimization systems. *Comput. Chem. Eng.* **20**(6), pp. 717–734.

Koninckx, J. (1988). On-Line Optimization of Chemical Plants Using Steady-State Models. PhD thesis. University of Maryland. College Park, MD.

MacGregor, J. F. and T. Kourti (1995). Statistical process control of multivariate processes. *Control Eng. Practice* **3**(3), pp. 403–414.

Miletic, I. P. and T. E. Marlin (1998). On-line statistical results analysis in real-time operations optimization. *Ind. Eng. Chem. Res.* **37**(9), pp. 3679–3684.

Zhang, H. and P. D. Roberts (1991). Integrated system optimization and parameter estimation using a general form of steady-state model. *Int. J. Systems Sci.* **22**(10), pp. 1679–1693.