Move Moderation in Real-Time Optimization Systems

Laura L. Ronholm and Thomas E. Marlin
Department of Chemical Engineering, McMaster University, Hamilton, Ontario, Canada L8S 4L7

Abstract

Real-time optimization of plant operations can be implemented in closed-loop, without operator intervention required. In this case, the optimizer selects the size and direction of changes to plant operation. Systematic analyses of optimization results are required prior to plant implementation. This paper presents a method for moderating the magnitude of the changes, while retaining the good tracking capability of the closed-loop system. The method involves an optimization to tradeoff the size of the move with the profit gained, along with constraints to ensure rapid achievement of the plateau on the profit contour. Many case studies with various disturbances, model mismatch, and measurement errors confirm that the method provides improved performance with flexibility for many scenarios.

1.0 Introduction

Real-time operations optimization (RTO) is an attractive method for increasing the profit of a chemical plant (Marlin and Hrymak, 1997; Cutler and Perry, 1983; Darby and White, 1988). The opportunities addressed in this paper involve model-based, closed-loop, optimization of operating variables in a continuously operating plant. The system considered is restricted to steady-state optimization in which the disturbance period is long compared with the plant dynamics.

RTO systems are designed to track the changing optimum operation in a plant as disturbances occur. In deciding when and how to change the plant operation, we have two major considerations. On one hand, moving the conditions quickly enable us to realize high profit, if the RTO system is accurately and consistently predicting the best conditions. On the other hand, following an inaccurate, noisy prediction will not increase, and can decrease, the average plant profit; this issue has been addressed by previous research that evaluates the confidence of the prediction (Miletic and Marlin, 1998). In addition, moving the plant a large amount in one step will cause large transients during which the plant might be disturbed, so that product qualities deviate from desired values. In this paper, a new technique to *moderate* changes to plant operation is presented that finds the best tradeoff of move size and profit increase.

2.0 Elements of the RTO Loop

Before this new technique is explained, we introduce the RTO loop, the components of the loop, and the interaction among these components. These RTO components define the technology which will be enhanced by the new technique and against which improvements in performance will be evaluated. It is necessary to understand the details of these components in order to understand the full effect of the move moderating technique. A typical RTO system is shown in Figure 1. The three major elements are the model updating, profit optimization, and results analysis. Each is discussed briefly in the subsequent sub-sections.

2.1 Model Updating

Model updating includes steady-state detection, gross error detection and parameter estimation. Since this technique will function with any technology for the first two of these, the discussion will concentrate on the parameter estimation, which calculates selected parameters ($\boldsymbol{\beta}$) based on measurements from the plant ($\mathbf{z}$). The parameter estimation method commonly used involves error-in-variables estimation applied to models that are non-linear in the parameters. A frequently used formulation is referred to as data reconciliation and parameter estimation (DRPE), and its formulation is given in the following.

$$\begin{aligned} \min_{\boldsymbol{\beta},\mathbf{a}} \quad & \phi(\mathbf{a},\boldsymbol{\beta}) = \mathbf{a}^{\mathrm{T}}\mathbf{S}^{-1}\mathbf{a} \\ \textbf{s.t.} \quad & \mathbf{h}(\mathbf{x}_{\mathrm{v}},\boldsymbol{\beta}) = 0 \\ & \mathbf{z} = \mathbf{A}\mathbf{x}_{\mathrm{v}} - \mathbf{a} \end{aligned} \tag{1}$$

In the above equation, **h** represents the nonlinear material and energy balance equations that represent the plant, **A** is a square and diagonal incidence matrix that accounts for the measurements of the model variables, **S** is a matrix of the measurement variances, and $\mathbf{x}_{\mathrm{v}}$ is the augmented vector of independent and dependent optimization variables.

2.2 Profit Optimization

The operating profit includes contributions from feed purchase, product sales, energy consumption, solvent loss, and other factors that are influenced by the operating variables; it does not include fixed costs like capital purchases or labor. The plant must be operated in a safe manner that produces on-specification products within a specified range of production rates. When additional degrees of freedom are available after these objectives are satisfied, optimization is possible. The optimization is defined in the following.

$$\begin{aligned} \max_{\mathbf{x}} \quad & \mathrm{Profit}(\mathbf{x},\mathbf{u},\boldsymbol{\beta}) \\ \text{s.t.} \quad & \mathrm{h}(\mathbf{x},\mathbf{u},\boldsymbol{\beta}) = 0 \\ & \mathrm{g}(\mathbf{x},\mathbf{u},\boldsymbol{\beta}) \geq 0 \\ & \mathbf{x}_{\mathbf{min}} \leq \mathbf{x} \leq \mathbf{x}_{\mathbf{max}} \end{aligned} \tag{2}$$

In the above equation, **x** and **u** are the independent and dependent optimization variables, respectively, while **h** and **g** represent the equality and inequality constraints of the plant. The result of this problem is a set of values for the optimization variables (**x**), which are typically set points for controllers.

2.3 Results analysis

Both practitioners and researchers have recognized the disadvantages of implementing every optimization result, because of (1) noise propagation in the RTO loop, (2) ill conditioning in the updater (3) ill conditioning in the optimizer, and (4) upsets to the plant operation.

Current industrial practice reduces the RTO move by constraining the optimization variables within a small “trust region”, which defines the allowable change in plant operation for one RTO execution. In addition, a minimum profit increase is required for operation to be changed. This approach can yield a poor initial direction, and it could fail to track a significant change if the gradient in the region around the current operation is very small.

Previous research results have applied a statistical test that allows implementation only when the new optimization result (operating conditions) are significantly different from the current plant operation (Miletic and Marlin, 1998). This statistical approach requires that the effect of common cause variability of measurement noise and high frequency disturbances on the results of equations (1) and (2) be determined. This has been accomplished by using linear approximations of the sensitivities to determine the variance propagation. This approach has moderated the RTO results, especially for factors (1) and (2) given above. However, the RTO results can still move too aggressively, for example, by “sliding” along a profit ridge.

3.0 New move moderation technique

In this section, a new method to moderate the magnitude of moves in an RTO system is described that can make the transition between operating points more gradual. This method is applied after the statistical test on the calculated set points has been performed and a significantly different operating point has been detected. The move moderating technique is shown in the dashed box in Figure 1. The subsequent analysis in the move moderation component trades off the increase in profit and the size of the change of operating variables, while ensuring that the move still remains statistically significant. This approach will be especially effective when the profit contour has a plateau with nearly constant profit over a range of operating conditions in the same direction.

Since the move moderation determines a compromise between immediate profit and move size, it can be naturally posed as an optimization problem. We introduce the problem in a stepwise manner, the objective function first and then the constraints individually.

- **Objective function** – The tradeoff is posed as a "move suppression" similar to the typical method used in some MPC controllers (Garcia, et al, 1989). The following equation defines how the sum of the profit difference from the predicted new optimum is balanced with the size of the move from the current to predicted new operating condition.

$$\theta_{mm}\left\{\left(\mathbf{x}_{mm}(1)-\mathbf{x}_{p}(1)\right)^2+\left(\mathbf{x}_{mm}(2)-\mathbf{x}_{p}(2)\right)^2\right\}+\left(\mathrm{Profit}_{m}-\mathrm{Profit}_{mm}\right)^2 \tag{3}$$

The parameter θ_{mm} is specified by the user and is essentially a tuning parameter for the method. In the above equation, the subscript mm represents the values at the move-moderated set point, p represents the values at the current set point, and m represents the estimated value the model optimum.

- **Plant model constraints** – The relationship between the operating conditions and the profit requires that the plant model be evaluated. Since the subsequent case study includes only equality constraints, we show only those in the following, which are evaluated at the move-moderated operating conditions.

$$h(\mathbf{x}_{mm},\mathbf{u},\boldsymbol{\beta})=0 \tag{4}$$

- **Statistically significance constraint** – We want to ensure that the new operating conditions are statistically significant from the current point, *after* the move moderation. Therefore, we ensure that the multivariate confidence intervals do not overlap. This requirement imposes a constraint based on the Hotelling T^2 statistic, which is given in the following equation.

$$\left(\mathbf{x}_{mm}-\mathbf{x}_{p}\right)^{T}\mathbf{Q}_{\mathbf{x}}^{-1}\left(\mathbf{x}_{mm}-\mathbf{x}_{p}\right)>\mathrm{UCL} \tag{5}$$

In the above equation, $\mathbf{Q}_x$ is an estimate of the covariance matrix of the optimal optimization variables. The control limit (UCL) would be tuned based on plant experience with common cause noise propagation.

- **Profit constraint** – We might want to place a constraint on the maximum reduction in profit allowable in one step through move suppression. This would place a bound on the decrease in profit from the new optimum and the move-moderated operating conditions, as stated in the following.

$$\mathrm{Profit}_{m}-\mathrm{Profit}_{mm}<\Delta\mathrm{Profit}_{max} \tag{6}$$

- **Profit ridge constraint** – Since we seek a move in a direction that gains the most profit for a limited magnitude, a good location would be along a ridge on the profit surface. This ridge is defined by a singular variable decomposition of the local Hessian approximation, which is calculated at the predicted new optimum operating conditions. The singular vector associated with the smallest singular value defines the direction of lowest slope, i.e., a ridge on the profit surface. The move-moderated operating conditions should lie on a line through the predicted maximum and along the direction of the singular vector. The constraint can be posed as given in the following equation.

$$\frac{\left(\mathbf{x}_{mm}(1)-\mathbf{x}_{m}(1)\right)}{\left(\mathbf{x}_{mm}(i)-\mathbf{x}_{m}(i)\right)}=\frac{\mathbf{r}(1)}{\mathbf{r}(i)}\qquad \text{for } i=1 \text{ to } n \tag{7}$$

The optimization variables should be scaled using expected ranges of change of each before performing the singular value decomposition. Equation (7) is included for problems that exhibit strong directionality in the profit contours. Should a problem have a symmetric profit surface, equivalent performance of the move moderator might be obtained without the constraint in equation (7).

In summary, the new move moderation solves an optimization problem that minimizes equation (3) subject to equations (4) to (7). The results are a set of operating conditions ($\mathbf{x}_{\mathbf{mm}}$) that captures "much" of the possible profit increase while moderating the size of the move in a single RTO execution.

4.0 Reactor case study

The performance of the move moderation technique was tested using a simulation of a modified form of the continuous chemical reactor, shown in Figure 2, originally developed by Williams and Otto [1960]. Two reactant streams, F_A and F_B, are fed to the reactor, where three irreversible elementary reactions occur. The resultant product stream contains two desirable products, P and E, and two waste products, C and G, in addition to any unused reactants. The flow rate of reactant A (F_A) and the volume of the reactor are held constant, resulting in two independent optimization variables: the flow rate of reactant B (F_B) and the temperature of the reactor (T). These two optimization variables are manipulated to maximize the operating profit. The model is adjusted to the changing conditions by updating the three reaction rate parameters.

The purpose of the move moderation is to reduce the magnitude of the moves in the operating points of the plant, while at the same time achieving a profit that is close to the optimum value. Thus, the effectiveness of the move moderation was determined by examining the frequency of large moves and the integrated profit.

4.1 Performance of Move Moderator under the Influence of Plant Disturbances

The disturbances used to test the performance of the move moderation technique included a step disturbance in the reaction rate, a slow decay in the reaction rate, measurement errors, feed stream impurities, and noisy data. The step disturbance and slow decay in the reaction rate tested the ability of the system to handle sudden and gradual changes in the optimum operating point. The measurement errors tested the ability of the system to handle bias errors in the sensors. The feed stream impurities and model structure mismatch tested the ability of the system to handle an incorrect model of the plant. The noisy data tested the performance of the system with a poorly tuned critical limit for the hypothesis test (Type I error).

In each of the disturbance scenarios investigated, the move moderation greatly reduced the number of large moves while resulting in increased or only very slightly decreased profit. The effects on movements are illustrated in Figure 3 for a typical case, a step disturbance in the reaction rate with noisy measurement data. Full details are reported for all cases in Ronholm (2000).

4.2 Influence of Hypothesis Test on Move Moderation

To determine the effects of the results analysis hypothesis test on the move moderation, the base case system was simulated with the hypothesis test removed for a step disturbance in the reaction rate. The results indicated that the move moderation greatly reduced the number of large moves; however, a small but statistically significant profit loss occurred. When the weighting of the size of the move in relation to the loss in profit was retuned, excellent results were obtained.

4.3 Effect of Missing Measurements on Move Moderation

When an RTO system is running online, all of the measurements might not be available due to sensor failure. Two different situations were investigated with the Williams-Otto reactor in which selected exit composition measurements were missing. In each instance, the missing measurements were treated as additional parameters to be estimated in the parameter updater since these measurements were not available at the time of the RTO execution. The results indicated that the frequency of large moves actually increased for both scenarios of missing measurements, while the number of total moves decreased. Likely, this indicates that the results analysis hypothesis test was not allowing the changes in the operating point of the plant, causing the frequency of moves to decrease significantly. Further simulations were performed with the hypothesis test removed. The number of large moves was dramatically reduced, and the profit was not reduced.

4.4 Effect of Conditioning of the Hessian of the Profit Function on the Performance of the Move Moderation

One of the constraints included in the move moderation algorithm is that the move be confined to the direction of the ridge of the profit function since the profit is less restrictive to errors along this ridge. A ridge results when the Hessian of the profit function has strong directionality. Thus, conditioning of the Hesssian could potentially have an effect on the performance of the move moderator. Three different cases with varying levels of conditioning were simulated by adjusting the flow rate of A into the reactor. The results indicated that the move moderator is most effective for those cases that were poorly conditioned. For these conditions, the number of large moves was decreased dramatically. However, the frequency of large moves were also reduced in the well-conditioned case, although these effects were not as pronounced as they were in the cases with poor conditioning.

4.5 Influence of Model Mismatch on Performance of Move Moderator

Model mismatch occurs inevitably as a result of using the simplified or reduced models in RTO. To investigate the influence of model mismatch on the performance of the move moderator, cases were run with an RTO two-reaction model of the Williams-Otto (three reaction) plant for step disturbances in the reaction rate parameter. The results indicated that although the move moderator reduces the frequency of large moves, the profit is much less than the optimum. Further simulations were performed with the hypothesis test removed. The results showed a large improvement in the attained profit, indicating that the hypothesis test was causing the system to become “stuck” at a sub-optimal operating point. In these situations, either the hypothesis test should be removed or the control limits for the hypothesis test should be relaxed in order to obtain adequate performance.

4.6 Effect of Different Weightings in the Move Moderator

In some instances, the magnitude of change in one variable is more important than the combined magnitude of change in all variables. This may occur when it is more costly to make a change to the setting of one variable or when it is difficult to make changes in one of the variables due to resource or physical constraints. The move moderator presented in this paper can be easily adapted to reflect such cases by placing different weightings on the individual variables in the objective function. Simulations were performed in which the weightings for the optimization variables were adjusted and step disturbances in the reaction rate were introduced into the system. The frequency of large moves in the selected variable was reduced without causing any significant decrease in profit.

5.0 Conclusions

A method has been presented in this paper to moderate the moves in the operating points of the plant performed well in the cases investigated with the Williams-Otto reactor. In the cases investigated in this research, the move moderator reduced the frequency of large moves without significantly affecting profit.

Several cases demonstrated the separate effects of the two elements for RTO results analysis, hypothesis test and the move moderation. We recommend that both be retained. The hypothesis test can “catch” severe ill-conditioning, while the move moderation can prevent frequent moves of large magnitude. The case studies clearly reinforced the need for carefully tuning the hypothesis test and move moderator for the specific implementation; when both results analysis methods are present, the upper control limit on the hypothesis test can be increased, to make it somewhat less restrictive.

The move moderating technique was also shown to be very adaptable. The structure of the move moderator can be altered to reflect situations in which it is more costly or difficult to change one of the optimization variables by applying separate tuning for each manipulated variable.

The cost for achieving this improved performance is an additional optimization calculation in the RTO loop. With the improved numerical methods and computing speed, the calculation should not impede the application of this method.

6.0 References

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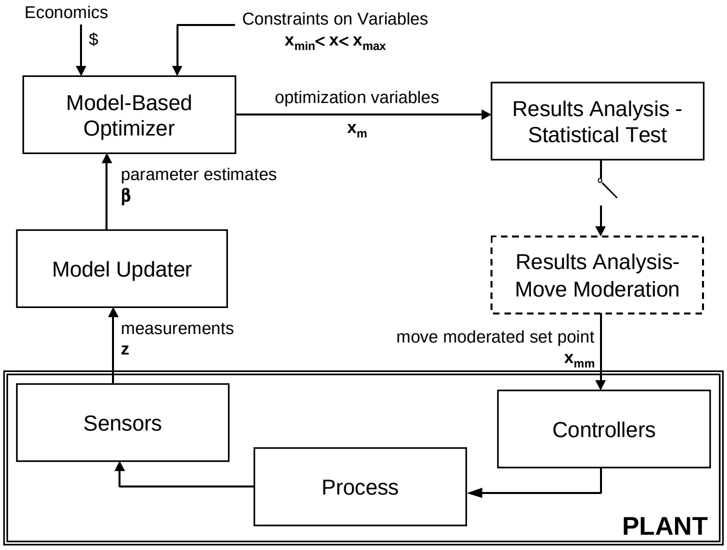

Figure 1. RTO loop elements.

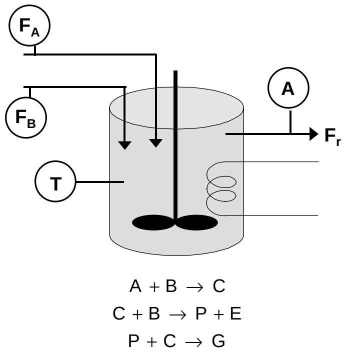

Figure 2. Schematic of Williams-Otto reactor.

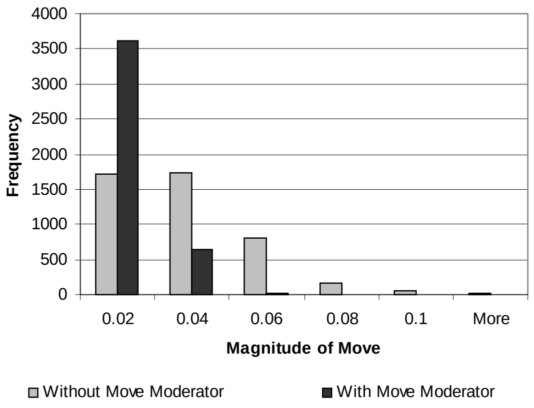

Figure 3. Effect of move moderation on the frequency of large moves.