15th Triennial World Congress, Barcelona, Spain

EVALUATION OF MEASUREMENT-BASED OPTIMIZATION SCHEMES FOR BATCH DISTILLATION

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Abstract: The standard approach to deal with uncertainty in dynamic optimization is to take a conservative stand. Measurement-based optimization schemes allow reducing this conservatism by using measurements to compensate for the uncertainty. On the example of productivity optimization of a batch distillation column with a terminal quality constraint, various measurement-based optimization schemes are compared. They all use measurements to update the input either from batch-to-batch or within the batch. A novel mid-course correction scheme for satisfying the terminal constraint is proposed. *Copyright © 2002 IFAC*

Keywords: Dynamic optimization, Batch distillation, Batch processes, Batch-to-batch optimization, Run-to-run Optimization, On-line optimization.

1. INTRODUCTION

The optimization of batch processes has received increasing attention since it is a natural choice for maximizing productivity. Typically the quantity of desired product is maximized at final time while respecting operational path constraints and terminal quality constraints. The classical approach is to apply open-loop input profiles that have been determined off-line. In practical applications, model mismatch and perturbations are present, which may lead to constraint violation or non-optimal operation. To satisfy the constraints despite uncertainty, conservative input trajectories that guarantee feasibility are sought (Terwiesch *et al.*, 1994). However, such a conservative strategy is, in most cases, non-optimal.

When suitable measurements are available, they can be used in the optimization scheme to reduce conservatism (Bonvin *et al.*, 2001). Depending on the availability of measurements, the inputs are updated during the batch (intra-batch) or in a batch-to-batch manner (inter-batch). The intra-batch optimization is capable of coping with perturbations that occur during a batch run. The objective of inter-batch optimization is to exploit the repetitive nature of batch processes to find the optimal operating conditions iteratively.

Two approaches can be distinguished depending on whether or not the model is used at the implementation level (Srinivasan *et al.*, 2002). When a model is used for implementation (indirect approach), updated optimal trajectories are computed using the estimates of the states and/or parameters. When the model is not used in a run-to-run scheme (direct approach), the input parameters are updated by a feedback controller to meet the terminal constraints (Srinivasan *et al.*, 2001). With on-line measurements, the direct approach requires a mid-course correction strategy to satisfy the terminal constraints (Yabuki and MacGregor, 1997). This paper proposes a novel scheme that tracks an off-line determined trajectory.

As an example, the optimal operation of a batch binary distillation column is studied. Numerous publications deal with the optimization of batch distillation columns for the case of no uncertainty (Hansen and Jørgensen, 1986; Diwekar *et al.*, 1987; Farhat *et al.*, 1991). The objective is to maximize the quantity of distillate at final time, or to minimize the time of operation for a given productivity. Typically, a terminal constraint on the average distillate quality is imposed. Fewer articles deal with the optimal operation of batch distillation columns under uncertainties. To compensate for uncertainties in the feed composition, it was proposed to choose off-line computed optimal trajectories based on temperature measurements in the initial startup phase (Barolo and Dal Cengio, 2001). The tracking of optimal temperature profiles was applied to a reactive batch distillation in order to prevent the breakthrough of the light component into the distillate (Sørensen *et al.*, 1994).

In this paper, the problem of maximizing productivity with a terminal constraint on quality will be studied with the reflux ratio being the sole manipulated variable. Various measurement-based optimization schemes will be evaluated in the presence of uncertainty in the relative volatility and boilup rate, with the measurement of the average distillate composition used to compensate for the uncertainty.

This paper is organized as follows. In the next section, a classification of optimization schemes to deal with uncertainty is undertaken. Section 3 describes the on-line tracking scheme that can be used for tracking terminal constraints. The problem of optimizing a distillation column is presented in Section 4, and various optimization schemes are evaluated on this example in Section 5. Finally, conclusions are drawn in Section 6.

2. CLASSIFICATION OF OPTIMIZATION SCHEMES

The terminal-cost optimization problem with uncertain parameters θ, perturbations $d^k(t)$ and measurement noise v^k in the k^{th} batch can be stated formally as follows:

$$\begin{aligned} \max_{u^k(t)} \; & J^k = \phi(x^k(t_f), \theta) \qquad (1) \\ s.t. \quad & \dot{x}^k = F(x^k, u^k, \theta) + d^k(t), \; x^k(0) = x_0^k \\ & S(x^k, u^k, \theta) \le 0, \quad T(x^k(t_f), \theta) \le 0 \\ & y^k = h(x^k, \theta) + v^k(t) \\ given \quad & z^j, \quad \forall\, j = \{1 \ldots k-1\} \\ or \quad & y^k(t_i), \quad \forall\, i = \{1 \ldots l\} \end{aligned}$$

where J^k is the cost function, u^k the inputs, x^k the states with initial conditions x_0^k, $S(x^k, u^k, \theta)$ the path constraints, and $T(x^k(t_f), \theta)$ the terminal constraints. The measurements at the end of the j^{th} batch are represented by z^j, $j = \{1 \ldots k-1\}$, and $y^k(t_i)$ represents the on-line measurements at time instant t_i in batch k.

In the presence of uncertainty, the introduction of a security margin (backoff) for active constraints is necessary. Backoffs ($b_S \ge 0$, $b_T \ge 0$) can be added to the path and terminal constraints: $S(x^k, u^k, \theta) + b_S \le 0$, $T(x^k(t_f), \theta) + b_T \le 0$. The backoffs are so chosen that the probability of constraint satisfaction is larger than a pre-specified confidence level. Since the backoffs affect the optimal solution, which in turn affects the backoffs, the backoffs have to be calculated using an iterative scheme (Srinivasan *et al.*, 2002).

Different dynamic optimization schemes are classified in Figure 1 (Bonvin *et al.*, 2001). Possible combinations of the schemes are not considered, whereby certain parameters are adapted on-line and others on a batch-to-batch basis.

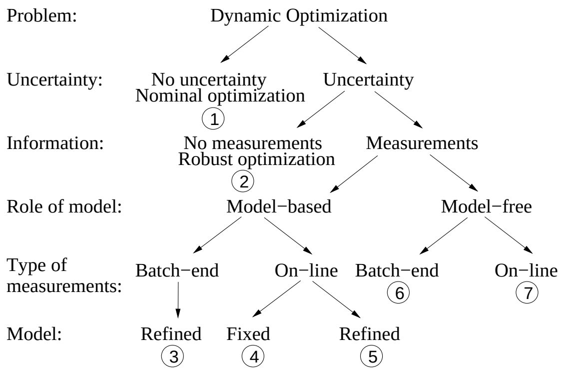

Fig. 1. Classification of dynamic optimization schemes in the presence of uncertainty (the numbers correspond to the schemes tested in this work)

2.1 Nominal optimization

When uncertainty is neglected, the nominal or expected values of the uncertain parameters are used in the optimization. Thus, the nominal solution may not even be feasible, let alone optimal, in the presence of uncertainty.

2.2 Robust optimization

By taking the uncertainty into account explicitly, a robust solution is obtained, for example by considering the worst-case scenario for the constraints and optimizing the cost in an expected sense. Such a conservative solution guarantees feasibility, however the cost is inferior due to the introduction of backoffs.

2.3 Batch-to-batch optimization, refined model

When measurements are available at the end of the batch, they can be incorporated into an optimization scheme that updates the input trajectories in a batch-to-batch manner. The optimization

scheme consists of two steps:
(i) estimation of the uncertain parameters at the end of each batch, and
(ii) computation of the optimal input trajectories using the refined model.
Both steps use the model explicitly and can become computationally expensive with large models. Additionally, a conflict between identification and optimality objectives may be observed (Srinivasan *et al.*, 2002): If the input it not sufficiently excited, it may not be rich enough to uncover the uncertain parameters. On the other hand, if the input is sufficiently excited, the operation may no longer be optimal.

2.4 On-line optimization, fixed model

When measurements are available during the batch, reoptimization can be executed with the advent of every measurement. It is supposed that reoptimization can be completed in-between the measurements, so that the inputs are updated after each measurement. When a fixed model is used, only the states are estimated and the optimal trajectory is calculated for the remaining of the batch. However, due to model inaccuracies, the computed optimal solution can become infeasible, especially towards the end of the batch.

2.5 On-line optimization, refined model

To compensate for the model inaccuracies, the uncertain parameters can also be estimated online using the available measurements. The estimated parameters are then used in a refined model for the calculation of the optimal trajectory from current time until terminal time. When such an approach is used, the system might not be sufficiently excited.

2.6 Batch-to-batch optimization, model-free

In model-free implementation schemes, the measurements are used directly to adapt the optimal input. They use the fact that the optimal inputs of (1) consist of various arcs and the inputs can be parameterized as a function of the states and so-called input parameters π, $u = \mathcal{U}(x, \pi)$. The input parameterization also includes the switching time between different arcs.

Without loss of generality, assume that all terminal constraints are active. Then, the necessary condition of optimality with parameterization π can be stated as follows (Srinivasan *et al.*, 2002):

$$T = 0, \quad \psi = \frac{\partial \phi}{\partial \pi} + \nu^T \frac{\partial T}{\partial \pi} = 0 \qquad (2)$$

where ν is the vector of Lagrange multipliers for the terminal constraints. The idea of model-free optimization is to satisfy the necessary conditions of optimality (2) despite uncertainty by adjusting the values of π using measurements. The necessary conditions consist of two parts: (i) the constraint part $T = 0$, and (ii) the sensitivity part $\psi = 0$. Since there is usually considerably more to gain by meeting the constraints than from reducing the sensitivities to zero, only the satisfaction of terminal constraints will be discussed in this paper.

Let (i) the batch-end measurements correspond to the terminal constraints, $z^j = T(x^j(t_f))$, (ii) a subset of π, $\bar{\pi}$ of dimension τ, have a large influence on T, and (iii) the $\tau \times \tau$ gain matrix, $G : \bar{\pi} \to z$, relate the input parameters $\bar{\pi}$ to the measurements z. Then, G^{-1} can be used for decoupling, with the following update law for $\bar{\pi}$:

$$\bar{\pi}^{j+1} = \bar{\pi}^j + G^{-1} K^j z^j \qquad (3)$$

This represents an integral control law, where K^j is a diagonal gain matrix of dimension $\tau \times \tau$. The other elements of π are kept constant.

2.7 On-line optimization, model-free

In the previous subsection, a batch-to-batch adaptation methodology that uses batch-end measurements for pushing the system closer to terminal constraints was presented. However, when on-line measurements are available, a mid-course correction methodology to satisfy terminal constraints is necessary. One such scheme will be discussed in the next section.

3. ON-LINE TRACKING TO MEET TERMINAL CONSTRAINTS

With batch-end measurements, only variations that occur the same way in every batch can be compensated. On-line measurements, on the other hand, can be used to handle a larger class of uncertainties within the batch, so that the backoff can be reduced.

Since the goal is to be as close to the terminal constraints as possible, the needed batch-end measurements correspond to the terminal constraints. Since on-line measurements do not directly provide this information, some sort of prediction or extrapolation is needed. Such a prediction is not always accurate due to model mismatch and disturbances. Though model mismatch can be handled by refining the model using measurements, the approach typically suffers from lack of persistent excitation.

Suppose the on-line measurements $y(t_i) = T(x(t_i))$ are available, i.e., the quantities corresponding to the terminal constraints $T(x(t_f))$ are not only measured at the end of the batch but also during the batch. The idea proposed in this paper is to track a conservative reference trajectory $y_r(t)$ whose main purpose is to guarantee the satisfaction of the terminal constraints at final time, i.e., $y_r(t_f) = 0$. Then, the adaptation law is given by:

$$u(t_i) = u_r(t_i) + K_p(y_r(t_i) - y(t_i)) \tag{4}$$

where u_r and y_r are the reference input and output trajectories. The inputs are constant between sampling instants. Optionally, an integral term can be added to the adaptation law (4). Also, reference trajectories with $y_r + b_T \leq 0$ can be chosen to provide a safety margin in the presence of measurement noise.

Though this scheme does not use the model for implementation, a model is needed to generate the reference trajectories. If there is no uncertainty (modeling errors and disturbances), then $y(t_i) = y_r(t_i)$, and the proposed feedback controller has no effect, $u(t_i) = u_r(t_i)$. In comparison to tracking a state variable (Sørensen *et al.*, 1994), the role of the feedback controller is not to steer the system towards a desired state, but towards the terminal constraints $y_r(t_f) = 0$, thereby rejecting the effect of model uncertainty and disturbances.

It is interesting to note the twist in concept – the model is not adapted to provide a good prediction of the system behavior, instead, the inputs are adjusted for the system to follow the model prediction. Since the model prediction renders the terminal constraints active, following it close enough will push the system towards the terminal constraints.

Note that no optimization nor estimation has to be executed on-line, which makes this method computationally attractive and numerically robust. So, in comparison to the model-based online optimization scheme, the sampling frequency can be higher, the backoff reduced, and the cost improved.

4. OPTIMIZATION OF A BATCH BINARY DISTILLATION COLUMN

4.1 Modeling

The model is based on previous work reported in the literature, see e.g. (Hansen and Jørgensen, 1986), (Diwekar *et al.*, 1987) and (Farhat *et al.*, 1991). The following assumptions are made: (1) Equimolar overflow, (2) Constant relative volatility and ideal vapor-liquid equilibrium, (3) Equilibrium stages, (4) Negligible vapor holdup, (5) Constant liquid holdup on stages and in condenser, (6) Total condenser, (7) Constant boilup rate.

Considering a column with a total of p equilibrium stages, the following model of order $(p + 2)$ is obtained:

$$\dot{M}_1 = -f_d V \tag{5}$$

$$\dot{x}_1 = \frac{V}{M_1}\left(x_1 - y_1 + (1 - f_d)\, x_2\right) \tag{6}$$

$$\dot{x}_i = \frac{V}{M_i}\left(y_{i-1} - y_i + (1 - f_d)\,(x_{i+1} - x_i)\right) \tag{7}$$

$$\dot{x}_c = \frac{V}{M_c}\left(y_p - x_c\right) \tag{8}$$

$i = 2, \ldots, p$, where x_i is the molar liquid fraction, y_i the molar vapor fraction and M_i the holdup on Stage i. Stage 1 refers to the reboiler and Stage p to the top of the column. The composition of the liquid flow entering the top stage corresponds to the composition in the condenser, x_c, i.e., $x_{p+1} = x_c$. M_c is the holdup in the condenser. The ratio f_d of the distillate to boilup rate, $f_d = \frac{D}{V}$, is considered as the manipulated variable. The vapor-liquid equilibrium relationship is:

$$y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i}, \quad i = 1, \cdots, p \tag{9}$$

where α is the relative volatility. The model parameters and the initial conditions are given in Table 1. The composition of the accumulated distillate, x_d, is assumed to be measured with the sampling time, t_s, and is given by:

$$x_d(t) = \frac{\sum_{i=1}^{p} x_i(t)M_i(t) - x_i(0)M_i(0)}{M_1(t) - M_1(0)} \tag{10}$$

Table 1. Model parameters and initial conditions, $i = 2, \cdots, p$

p	10		V	15	kmol/h
t_f	10	h	$x_{d,des}$	0.9	kmol/kmol
t_s	30	min	$M_1(0)$	100	kmol
α	1.5		$x_1(0)$	0.5	kmol/kmol
M_i	0.2	kmol	$x_i(0)$	0.5	kmol/kmol
M_c	2	kmol	$x_c(0)$	0.5	kmol/kmol

The objective is to maximize the quantity of accumulated distillate for a given batch time t_f with a terminal constraint on $x_d(t_f)$. Additionally, there are path constraints on the manipulated input f_d. The optimization problem is mathematically stated as follows:

$$\max_{f_d(t)} \; J = M_1(t_0) - M_1(t_f) \tag{11}$$

$$\begin{aligned} s.t. \quad & \text{Diff. Alg. Equations } (5) - (10) \\ & 0 \leq f_d(t) \leq 1 \\ & x_d(t_f) \geq x_{d,des} \end{aligned}$$

4.2 Characterization of the optimal solution

The optimal solution obtained numerically consists of three intervals:

(1) Full reflux ($f_d = 0$). Startup phase to increase the composition of the light component in condenser,

(2) A nearly linear arc to represent the compromise between quality and productivity,
(3) No reflux ($f_d = 1$) in order to empty condenser.

As a result, the input can be parameterized using the following four parameters: the two switching times t_1 and t_2 and the parameters for the linear profile, the initial level l and the slope s. The parameterized optimal input trajectory is illustrated in Figure 2. This parameterization results in the optimal cost $J = 22.73\ kmol$, and the input parameters are $\pi = [t_1\ t_2\ l\ s]^T = [1.02\ 9.88\ 0.1748\ {-0.0039}]^T$.

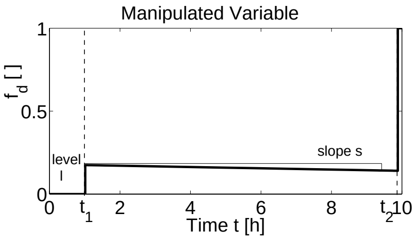

Fig. 2. Parameterization of the input f_d.

5. EVALUATION OF VARIOUS SCHEMES

In order to provide a realistic test scenario, the following uncertainty is considered:

- Parametric uncertainty: Constant but unknown relative volatility in the range $\alpha = [1.4\ 1.6]$
- Perturbation: Boilup rate uniformly distributed in the range $V = [13\ 17]\ kmol/h$, value changed every $2.5h$
- Measurement noise: Product composition x_d with 5% multiplicative gaussian noise

The value $\alpha = 1.5$ is used in all simulations. However, this value is not disclosed to the various optimization schemes that start with the worst-case value $\alpha = 1.4$. The costs are calculated on the basis of 50 realizations with respect to perturbation and measurement noise. Backoffs are introduced so that in every case the constraint satisfaction is 99%.

The results of the various optimization schemes are compared in Table 2. The loss in performance is calculated as: Loss $= (J_{nom} - J)/J_{nom}$, where J is the actual cost and J_{nom} the nominal cost without parametric uncertainty, perturbation and measurement noise. The input profiles could be updated either (i) on-line, (ii) batch-to-batch, or (iii) both. This latter case is not considered here. Thus, with on-line schemes, the improvement shown in Table 2 is that obtained over a single batch.

(1) Nominal case: When the nominal input trajectory is applied open-loop in the presence of uncertainty, the terminal constraint is satisfied in only 53% of the realizations.

Table 2. Comparison of cost and required backoff. The numbering refers to subsections of Section 2

	Method	Cost J [$kmol$]	Backoff b_T	Loss [%]
1	Open loop, nominal input	-	infeasible	-
2	Open loop, robust input	14.98	0.042	34.1
3	Batch-to-batch, refined model	20.32	0.015	10.6
4	On-line, fixed model	20.20	0.015	11.1
5	On-line, refined model	20.41	0.013	10.2
6	Batch-to-batch, model-free	20.83	0.012	8.4
7	On-line, model-free	20.64	0.010	9.2

(2) Robust case: If measurements are not available, constraint satisfaction is guaranteed by using the worst-case parameters in the optimization, $\alpha = 1.4$ and $V = 17\ kmol/h$.

(3) Batch-to-batch, refined model: In the batch-to-batch optimization scheme, the uncertain parameters are estimated by least-squares estimation using the batch-end measurements of average distillate composition. The refined model is then used to update the input parameters. The optimal cost is reached in about 5 batches (Figure 3), but the cost changes significantly from batch to batch due to the perturbation and measurement noise.

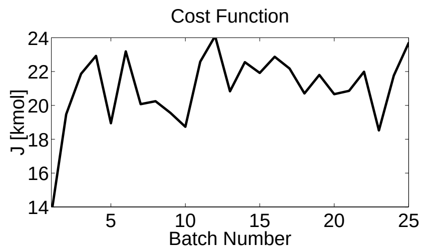

Fig. 3. Evolution of the cost function for the batch-to-batch, refined model scheme.

(4) On-line case, fixed model: If the measurement of x_d is available on-line, the current state of the system can be estimated and used for reoptimization. However, such a procedure is slightly inferior to batch-to-batch schemes due to inaccurate parameters. Also, the computed optimal input can become infeasible towards the end of the batch and the no reflux interval has to be eliminated to circumvent the problem.

(5) On-line, refined model: Here, the uncertain parameters are also estimated. The forgetting factor $\lambda = 0.94$ is used in the least-squares estimation. It was observed that the parameter estimates do not actually coincide with the true values. This can be attributed to bias in estimation, a lack of excitation, and infrequent measurements. Also, since the measurements are only available after

the switching time t_1, this input parameter cannot be adapted in any on-line optimization method.

(6) Batch-to-batch, model-free: Among the input parameters $\pi = [t_1, t_2, l, s]$, the switching time t_2 changes only marginally with the uncertainty considered and need not be adapted. The parameter with the strongest influence on the terminal quality constraint is the level l. So, a simple integral control law as in (3): $l^{j+1} = l^j + G^{-1}\ K^j\ T^j$, with $G^{-1} = 1.5$, is used for batch-to-batch optimization. In addition, the controller gain is reduced with the batch number j: $K^j = j^{-0.9}$. With such a scheme, the optimal cost is reached in about 5 batches (see Figure 4). Note that the variations in cost due to perturbation and noise are less than with the batch-to-batch, refined-model scheme (Figure 3).

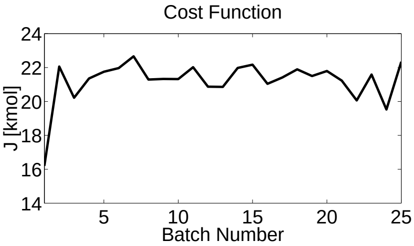

Fig. 4. Evolution of the cost for the model-free batch-to-batch scheme.

(7) On-line case, model-free: Assuming that $y(t_i) = x_d(t_i)$ can be measured without any delay, a trajectory $x_{d_r}(t)$ is tracked. In this case, the conservative trajectory computed off-line using robust optimization techniques. Here, trajectory tracking closely resembles the constant distillate purity method of operation. The backoff $b_T = 0.01$ is added to the reference trajectory, and tracking is done using an empirically tuned PI-controller with $k = 1.2, T_i = 1.6$. Figure 5 shows that though the reference trajectory is not perfectly tracked, the terminal constraint is attained at the end of the batch.

The performance could still be improved in two ways: (i) If the measurements are available more frequently, it is possible to decrease the sampling time, since on-line computation is minimal. With the sampling time $t_s = 3\ min$, the backoff can be reduced to $b_T = 0.009$ and the performance loss is only 7%. (ii) Performance improvement can be achieved with a combination of on-line tracking and batch-to-batch adaptation of the reference trajectory $x_{d_r}(t)$.

6. CONCLUSION

Several optimization schemes that use measurements to reduce conservatism (necessary in the presence of uncertainty) have been presented. The methods were applied to a simulated batch binary distillation column with terminal cost and path and terminal constraints. A novel scheme was proposed to track a reference trajectory online, the purpose of which is to bring the system to the terminal constraints. This method is numerically robust since no parameter estimation nor trajectory reoptimization is required on-line. Future work will investigate the application of the method to non-ideal multi-input systems including several terminal constraints.

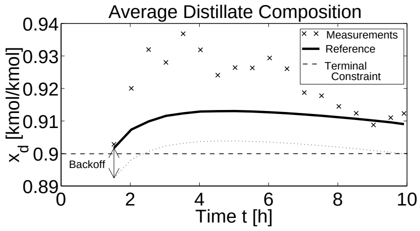

Fig. 5. Reference trajectory and measurements for the on-line model-free scheme.

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