2005 American Control Conference
June 8-10, 2005. Portland, OR, USA

Validation of a Solution Model for the Optimization of a Binary Batch Distillation Column

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Abstract— **For the optimization of dynamic systems, it is customary to use measurements to combat the effect of uncertainty. In this context, an approach that consists of tracking the necessary conditions of optimality is gaining in popularity. The approach relies strongly on the ability to formulate an appropriate solution model, i.e. an approximate parameterization of the optimal inputs with a precise link to the necessary conditions of optimality. Hence, the capability of a solution model to optimize an uncertain process needs to be assessed. This paper introduces an optimality measure that can be used to verify the conjecture that the solution model derived from a simplified process model can be applied to a more rigorous process model with negligible performance penalty. This conjecture is tested in a simulation of the dynamic optimization of a batch distillation column.**

Index Terms— **Dynamic optimization, Measurement-based optimization, Implicit optimization, NCO tracking, Batch distillation.**

I. Introduction

A frequent objective in batch process operation is the maximization of product yield at final time while satisfying path and terminal constraints. In the presence of uncertainty (model mismatch and/or process disturbances), the constraints are typically met by applying a conservative policy that, unfortunately, can be far from optimal. For process improvement and thus reduction of this conservatism, it is necessary to use measurements. This can be accomplished via model refinement and re-optimization (explicit optimization) or by updating the inputs directly (implicit optimization). This paper considers a technique of the latter class, i.e. optimization via tracking the necessary conditions of optimality (NCO).

NCO tracking treats the optimization problem as a feedback control problem, with the attendant advantages of sensitivity reduction and disturbance rejection [13]. Since the solution of a dynamic optimization problem is typically discontinuous and consists of various intervals, the NCO include several parts that correspond to meeting the active constraints and zeroing certain sensitivities, both during the run and at final time [1]. Some of these parts (conditions) can be enforced on-line, while the others need several successive runs to be met.

The NCO-tracking approach relies on the concept of *solution model*, which is a description of the input profiles from an optimality viewpoint, i.e. it relates the various elements of the optimal inputs to the NCO [11]. The solution model is based on the input trajectories obtained via numerical optimization of a nominal process model. Its construction involves input dissection, input parameterization and the generation of links between the input parameters and the different parts of the NCO. Input dissection consists of decomposing the input profiles into various intervals and identifying those elements that vary with uncertainty. Input parameterization is done so as to ease adaptation towards optimality. Finally, the input parameters are linked to the appropriate NCO.

An important issue in NCO tracking is the evaluation of the solution model's accuracy, i.e. its flexibility for approximating the optimal policy. In general, increasing the number of input parameters increases the accuracy and thus improves the objective function, but makes parameter adaptation more difficult [9], [4]. Also, different parameterization forms may lead to different levels of accuracy. An automated method for determining the various arcs and the switching times between them using multi-stage numerical optimization has been proposed recently [8]. This approach helps keep both the approximation error and the number of parameters small. The important problem of verifying whether the set of active constraints is invariant with respect to uncertainty has also been addressed recently [5]. Evaluating the accuracy of a given input parameterization has been an important topic in the numerical optimization literature, for which measures that use the adjoint variables have been proposed [2]. Yet, it has been suggested to use these measures as qualitative rather than quantitative indicators. In the same spirit, a simple optimality measure that expresses the loss with respect to truly optimal operation is proposed here.

A related issue is the solution model's applicability to the real process. Typically, the solution model is obtained through numerical optimization of a simplified tendency model. Hence, how can one assess whether the solution model also holds for a more rigorous process model and, hopefully, also for the real process? In this paper, this issue is tackled by comparing the value of the optimality measure for both a tendency model and a much more detailed model of the same process.

The fact that a solution model obtained from a simplified process model can be equally applicable to more rigorous process models will be illustrated in simulation via the optimization of a binary batch distillation column. The objective will be to determine the reflux ratio policy that maximizes the final distillate quantity while meeting a purity constraint on the distillate composition at a given final time. Numerous studies have considered the dynamic optimization of batch distillation columns. For binary systems, three different operating strategies can be distinguished [3]: a) constant reflux ratio, b) constant distillate composition, and c) optimal operation with time-varying reflux ratio. The latter strategy is considered in this study and includes the two former strategies as special cases. The same methodology can also be applied to reactive batch distillation columns [10].

This paper is organized as follows. Section II presents dynamic optimization via NCO tracking. This method requires an appropriate solution model, for the evaluation of which a measure of optimality is proposed in Section III. The dynamic optimization of a binary batch distillation column via NCO tracking is then illustrated in Section IV. The validation of appropriate solution models is also given therein. Finally, conclusions are drawn in Section V.

II. Dynamic Optimization via NCO Tracking

The idea of NCO tracking is to achieve optimality, also in the presence of perturbations, by treating the optimization problem as a control problem. Since process measurements are used, NCO tracking is robust with respect to uncertainty (model mismatch and process disturbances).

A. Problem Formulation

The terminal-cost optimization of dynamic processes with free terminal time and in the presence of path and terminal constraints is considered:

$$\begin{aligned} \min_{u(t),t_f} \quad & J = \phi(x(t_f)) \\ s.t. \quad & \dot{x} = F(x,u),\ x(0) = x_0 \\ & S(x,u) \leq 0, \quad T(x(t_f)) \leq 0 \end{aligned} \tag{1}$$

where ϕ is the scalar cost function, x is a vector of states with known initial conditions x_0, u is the input vector, and t_f is the final time. F are the functions describing the system dynamics, $S \leq 0$ the path constraints, and $T \leq 0$ the terminal constraints.

In general, the solution of problem (1) is discontinuous, consisting of a sequence of arcs or intervals [1]. Within each interval, the inputs are continuous and differentiable. The time instants at which the inputs switch from one arc to another are called *switching times*. Two different types of arcs can be distinguished: an input is either determined by an active path constraint (constraint-seeking arc) or is inside the feasible region (sensitivity-seeking arc).

B. Necessary Conditions of Optimality

Applying Pontryagin's Maximum Principle to (1) results in the following Hamiltonian and adjoint equations [1]:

$$H = \lambda^T F + \mu^T S \tag{2}$$

$$\dot{\lambda}^T = -\frac{\partial H}{\partial x}, \quad \lambda^T(t_f) = \left.\frac{\partial \Phi}{\partial x}\right|_{t_f} \tag{3}$$

where $\Phi = \phi + \nu^T T$ is the augmented terminal cost, $\lambda(t) \neq 0$ the adjoint states, $\mu(t) \geq 0$ the Lagrange multipliers for the path constraints, and $\nu \geq 0$ the Lagrange multipliers for the terminal constraints. The Lagrange multipliers μ and ν are nonzero when the corresponding constraints are active and zero otherwise so that $\mu^T S = 0$ and $\nu^T T = 0$ always [12].

The first-order necessary conditions of optimality can be written as

$$\frac{\partial H(t)}{\partial u} = \lambda^T \frac{\partial F}{\partial u} + \mu^T \frac{\partial S}{\partial u} = 0 \tag{4}$$

A free-terminal-time problem involves an additional condition, referred to as the transversality condition:

$$\frac{\partial \bar{\Phi}}{\partial t_f} = \left.\frac{\partial \Phi}{\partial t}\right|_{t_f} + H(t_f) = 0 \tag{5}$$

where $\bar{\Phi} = \Phi + \int_0^{t_f} H(t)\ dt = \phi + \nu^T T + \int_0^{t_f} [\lambda^T(t) F + \mu^T(t) S]\ dt$ is an augmented cost that includes both path and terminal components. The NCO can be partitioned by separating the active path conditions from the active terminal conditions on the one hand, and the constraint conditions from the sensitivity conditions on the other:

	Path	Terminal
Constraints	$\mu^T S = 0$	$\nu^T T = 0$
Sensitivities	$\frac{\partial H}{\partial u} = 0$	$\frac{\partial \bar{\Phi}}{\partial t_f} = 0$

(6)

The NCO include both path and terminal objectives, since there are conditions that have to be met during the operation while others need to be satisfied only at final time. Also, optimality implies keeping certain constraints active and forcing certain sensitivities to zero.

C. NCO Tracking

NCO tracking enforces the four components of (6), some on-line and the others over successive batches [12], [11]:

- The path constraints limit the values that the inputs or the states can take. Input bounds are straightforward to enforce. State constraints, which are typically key safety and operational limitations that are assumed to be measurable, can be enforced by on-line feedback control. On the other hand, path sensitivities are more difficult to implement since their evaluation requires a process model.

- The terminal constraints are typically kept active by measuring the constrained variables at final time and updating the inputs in the next run. The terminal sensitivities can be met on a run-to-run basis as well by estimating them using either a process model or measurements of the terminal cost.

It is helpful to parameterize the inputs using time functions and scalars that are assigned to the different components of (6). This assignment constitutes the *solution model*. In most cases, performance is insensitive to the form of the solution model, and this can be exploited to ease the adaptation and/or improve the performance [11].

The generation of a solution model involves the following three steps:

1) Determination of the switching structure of the optimal solution, i.e. the sequence and type of intervals present in the solution of (1). For this, numerical optimization of a nominal (tendency) process model is the method of choice. Arcs are typically detected by visual inspection, though an automated method for determining the switching structure has been proposed recently [8].

2) Determination of the input fixed and free variables. The elements of the inputs that are not affected by uncertainty are considered as fixed in the solution model and can be applied in an open-loop fashion, e.g. an input variable at its bound in a given interval. The input elements affected by uncertainty constitute the free (decision) variables of the optimization problem. These include time functions (arcs) and scalar values (switching times and, possibly, the final time t_f). Furthermore, since it is easier to deal with scalar values than with time functions, certain input arcs can be parameterized using a small number of parameters, e.g. using a piecewise-polynomial representation.

3) Linking the input free variables to the various parts of the NCO. The input fixed parts are known and can be implemented directly. In contrast, the input free variables need adjustment, and the NCO can be used for that purpose. The active path and terminal constraints determine certain arcs and parameters. The remaining decision variables are used to meet the path and terminal sensitivities. There is not a unique way of doing this assignment. Different pairings between the free variables on the one hand and the NCO parts on the other will imply different adaptation strategies. An important assumption for this assignment to be effective is that the set of active constraints is correctly determined and does not vary with uncertainty. Fortunately, this restrictive assumption can often be relaxed by considering a super-structure for the constraints [11].

The formulation of a solution model involves simplifications and approximations that help make the NCO-tracking problem more tractable and efficient. Simplifications can be introduced at various levels. For example, one can neglect arcs that contribute little to performance, or hold an input constant during a period in which it would otherwise change only slightly. Path sensitivity arcs can be approximated using piecewise-polynomial (e.g. piecewise-linear) or exponential functions.

III. Solution Model Validation

As described in the previous section, a solution model is a tool used to approximate the optimal inputs and allow their adaptation using measurements. There might be several solution model candidates for a given optimization problem. Hence, it is important to compare them and assess the quality of approximation. For this, an optimality measure is introduced next.

A. Optimality Measure

Let u^* be the true optimum, and u^s a candidate policy whose quality is to be determined. Also, let $J(u^*)$ and $J(u^s)$ be the corresponding cost functions evaluated on the real plant (or its representation in a simulation study).

A simple way of assessing the distance of the proposed solution to the true optimum is to define the loss function

$$\Theta_{loss} = \frac{J(u^s) - J(u^*)}{|J(u^s)|} \qquad (7)$$

which normalizes the difference $J(u^s) - J(u^*)$ with respect to the obtained cost $|J(u^s)|$. The absolute value is introduced here to normalize with a positive number since the cost function can be negative, e.g. upon transforming a maximization problem into the minimization formulation (1). Also, normalization helps compare optimality measures for different processes. The measure Θ_{loss} is positive or zero. Note that, for a maximization problem, one would use $J(u^*) - J(u^s)$ in the numerator of Θ_{loss}.

This optimality measure requires knowledge of the true optimal cost $J(u^*)$, which is typically not available in practical applications. Even in a simulation study, u^* is difficult to calculate since it necessitates an infinite-dimensional parameterization. However, in the absence of path constraints, a good approximation of the cost $J(u^*)$ – though not necessarily of the inputs u^* – can be obtained by increasing the number of parameters and extrapolating as in [6]. In the presence of path constraints, extrapolation will typically fail each time an additional constraint becomes active as the result of more flexibility in the inputs. Yet, when the set of active constraints does not change with additional input parameters, extrapolation can be made.

B. Robustness of the Solution Model

The optimality measure Θ_{loss} can be used to evaluate the quality of approximation of a given solution model. This section will investigate the robustness of the solution model by assessing whether the solution model that is derived from – and found appropriate for – a simple process model can be applied to different models of the same process with negligible loss in performance. It is important to realize that the robustness test is with respect to the solution model and not the optimal solution. In other words, though the optimal solution may vary significantly due to parametric and structural uncertainty, the link between the input free variables and the NCO that is used to achieve (near) optimality remains valid. The main conjecture addressed in this paper is presented next.

Conjecture : *A valid solution model is insensitive to "reasonable changes" in the plant model parameters and/or structure if the optimality measure Θ_{loss} remains close to zero.*

The conjecture can be understood as follows. Consider a process for which the two models $\mathcal{M}_1$ and $\mathcal{M}_2$ are available. Suppose the solution model $\mathcal{S}$ has been found appropriate for process model $\mathcal{M}_1$, i.e. $\Theta_{loss}(\mathcal{S}, \mathcal{M}_1) \simeq 0$. Then, if $\Theta_{loss}(\mathcal{S}, \mathcal{M}_2) \simeq 0$, the solution model $\mathcal{S}$ also holds for $\mathcal{M}_2$.

The conjecture says that the optimality measure Θ_{loss} (and not the cost function J) is insensitive to changes in the process model. In other words, if the solution model is adequate for optimizing correctly different models of the same process, Θ_{loss} remains nearly constant though J may change significantly. This indicates that the sequence of arcs and the associated input parameters are judiciously chosen and the solution model applies equally well to all process models. Conversely, if the optimality measure varies significantly in response to parameter and/or structural changes, the corresponding solution model is not appropriate.

C. Solution Model for the Real Plant

If the solution model has been found insensitive to "reasonable variations" in the plant model parameters and/or structure, one can then hope that the same carries over to the real plant. This is particularly true if these reasonable variations around the nominal plant cover the unknown real plant.

The following procedure is then proposed for generating and validating the solution model capable of optimizing a real plant:

1) Use a simple nominal plant model, generate the corresponding solution model, perform NCO tracking with it and compute the optimality measure Θ_{loss} using the nominal model as simulated plant.
2) Assess the amount of model mismatch between the plant model and the real plant and bound it in terms of parametric variations for the nominal model, i.e. determine one or several worst-case scenarios using the nominal plant model structure.
3) Using the same solution model, perform NCO tracking on these worst-case plant models and compute the associated optimality measures.
4) If all optimality measures are close to zero, the solution model is valid for all worst-case scenarios, i.e. hopefully also for the real plant. Otherwise, it is necessary to iterate and try to obtain a more detailed nominal plant model with reduced plant/model mismatch.

IV. Optimization of a Binary Batch Distillation Column

The above conjecture is tested on the batch distillation of a cyclohexane - n-heptane mixture. In this simulation study, the real plant is a packed column represented by an equilibrium stage model (see [14] for details). Briefly, this model assumes:

- negligible vapor holdup,
- perfect mixing,
- total condenser without sub-cooling.

Stage and condenser liquid holdups are modeled through weir equations. An energy balance on each stage governs the liquid temperatures. Vapor flow rates depend on pressure drop and thus differ from stage-to-stage. Composition- and temperature-dependent physical properties are used in the energy balance, liquid holdup and the pressure drop calculations. This process model, which will be referred to as the detailed process model, contains $3(p+1)$ differential equations, where $p = 20$ is the number of stages including the reboiler. Hence, the detailed column model is of 63^{rd} order.

On the other hand, a "tendency" model based on a shortcut method consists of only 3 differential equations, one each for the total reboiler holdup, the reboiler composition and the condenser composition. Assumptions include negligible stage holdup, constant condenser holdup and ideal vapor-liquid equilibrium. This tendency model, which is also described in [14], will be used to generate alternative solution models.

A. Problem Formulation

We restrict our attention to a problem in which the final time, t_f, is specified (e.g., the time available in one operating shift). The objective is to maximize the amount of distillate obtained, J, while meeting a purity constraint on the accumulated distillate composition x_D. The more volatile cyclohexane is the primary component of the distillate, and the remaining still bottoms is a solvent that may be discarded or recycled. The manipulated variable is the internal reflux ratio, $r(t)$, constrained between no reflux, $r = 0$, and total reflux, $r = 1$.

Increasing the internal reflux ratio improves the distillate purity but reduces its production rate. Thus, the optimal reflux profile will seek a compromise between quantity and quality. Conceptually, the reboiler duty and the column pressure are additional manipulated variables. However, maximizing production requires operation at the maximum pressure drop [7], which determines the reboiler duty. Furthermore, the separation of thermally degradable components calls for an upper temperature limit that fixes the maximal pressure. Without this limit, economic considerations would suggest operating the column at maximal pressure. Hence, the reboiler duty and the column pressure are not considered as manipulated variables here, but they are fixed at upper bounds related to maximal pressure drop and economic considerations (column design), respectively.

The above optimization problem can be expressed mathematically as follows:

$$\begin{aligned} \max_{r(t)} \ J \quad &= \quad \sum_{c=1}^{n}\sum_{i=1}^{p+1} H_{i,c}(0) - H_{i,c}(t_f) \qquad (8) \\ s.t. \quad & \quad \text{dynamic process model} \\ & \quad 0 \leq r(t) \leq 1 \\ & \quad x_D(t_f) \geq x_{D,des} \end{aligned}$$

where $H_{i,c}$ is the molar holdup of component c, $c = 1, ..., n$, on stage i, $i = 1, ..., (p+1)$. The total number of components is n (here $n = 2$), p is the number of stages including the reboiler ($i = 1$) and the condenser ($i = p+1$) . The amount of distillate at final time is expressed as the difference between the initial and final total holdups. The final time is fixed at $t_f = 3\ h$, and the desired final distillate composition is $x_{D,des} = 0.95\ kmol/kmol$.

B. Nominal Optimal Solution for Tendency Model

The optimal input trajectory is first computed by control vector iteration [3] for the tendency process model using 200 piecewise-constant elements. The resulting cost is $J = 1.327\ kmol$. The internal reflux ratio is initially $r = 1$, corresponding to full reflux (Figure 1). Then, the reflux ratio reduces to some intermediate value, and it becomes zero for a short time before the end of the batch. Extrapolation to the true optimal cost is possible in this case by computing the optimal input u^* analytically for each interval from the necessary conditions of optimality. The shape of the optimal input is very similar to that in Figure 1, and so is the optimal cost $J(u^*) = 1.327\ kmol$.

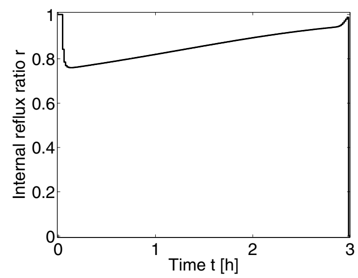

Fig. 1. Optimal piecewise-constant input trajectory with 200 elements for the tendency process model.

C. Various Solution Models

From visual inspection of the optimal input in Figure 1, the input profile can be divided into 3 intervals:

a) Startup phase with full reflux ($r = 1$)
b) Distillate withdrawal phase, intermediate reflux ($r \in [0, 1]$)
c) Condenser recovery phase, no reflux ($r = 0$)

This solution can be interpreted as follows: The full reflux interval corresponds to a startup phase, where the light component is accumulated in the condenser. After reaching a certain purity in the condenser (some value between $x_{D,des}$ and 1), distillate is withdrawn. Just before reaching final time, reflux is stopped for recovering the high-purity product present in the condenser.

Taking into account the presence of three intervals, the following solution model is first proposed (Figure 2). In Interval a, the reflux ratio is fixed to $r = 1$, followed by a linear profile with the values r_1 at t_1 and r_2 at t_2 in Interval b. Finally, the reflux ratio is fixed to $r = 0$ in Interval c. Upon fixing the reflux ratio in Intervals a and c, where input bounds are active, there are $N = 4$ input free parameters: t_1, t_2, r_1 and r_2. This model will be denoted as Solution Model A.

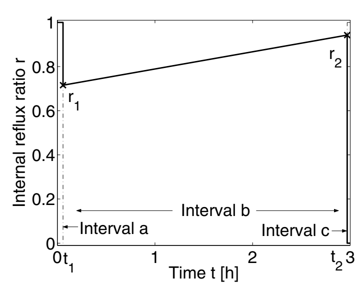

Fig. 2. Solution Model A with parameters t_1, t_2, r_1 and r_2.

The following alternative solution models will also be considered.

- In Solution Model B, the last interval is eliminated ($N = 3$, with the parameters t_1, r_1 and r_2).
- In Solution Model C, the reflux ratio is additionally kept constant in Interval b ($N = 2$, with the parameters t_1 and r_1).

D. Solution Model Evaluation

1) Comparisons for Tendency Model: The optimization results with the tendency model using different solution models are listed in Table I. It is seen from Θ_{loss} that a parameterization with only 4 parameters (Solution Model A) can be used to recover 99.8 % of non-optimality. The elimination of Interval c in Solution Model B barely affects the performance, while a constant reflux in Interval b (Solution Model C) causes significant deterioration in performance. Hence, Solution Models A and B can be considered as good approximations of the optimal solution since their optimality measures Θ_{loss} are close to 0.

TABLE I

REALIZED COST J AND OPTIMALITY MEASURE Θ_{loss} FOR THE TENDENCY PROCESS MODEL.

Strategy	J $[kmol]$	Θ_{loss}
True optimum (uncertainty known)	1.327	0
Solution Model A (NCO tracking)	1.325	0.002
Solution Model B (NCO tracking)	1.314	0.010
Solution Model C (NCO tracking)	1.223	0.085

Furthermore, it is interesting to note that, if a brute force piecewise-constant parameterization had been chosen, it would have required 180 parameters to match the performance of Solution Model A, 80 to match that of Solution Model B, and only 1 to match that of Solution Model C. This indicates that the input parameterization needs to include the switching instant t_1 and a non-constant reflux in Interval b.

2) Comparisons for Detailed Process Model: The Solution Models A-C generated using the tendency process model are now used to optimize the more detailed process model. The results are listed in Table II. Though the cost values are different from those in Table I, the optimality measures are similar. This indicates that the solution models exhibit about the same amount of approximation capability for both the tendency and the detailed process models. Hence, the solution models are rather robust with respect to plant/model mismatch and it seems reasonable to want to apply Solution Models A or B to the real plant.

TABLE II

REALIZED COST J AND OPTIMALITY MEASURE Θ_{loss} FOR THE DETAILED PROCESS MODEL.

Strategy	J $[kmol]$	Θ_{loss}
True optimum (uncertainty known)	1.399	0
Solution Model A (NCO tracking)	1.398	0.001
Solution Model B (NCO tracking)	1.374	0.018
Solution Model C (NCO tracking)	1.304	0.073

V. CONCLUSIONS

This paper has proposed an optimality measure for validating the input parameterization in the context of NCO tracking for dynamic optimization problems. Using this optimality measure, the applicability of a given solution model to different process models or uncertainty realizations can be assessed. A procedure has been proposed to validate the applicability of a solution model to a real plant.

The focus in this paper has been on comparing different solution models for optimizing two process models of widely different complexity developed for a binary batch distillation column. It has been shown that a solution model developed from a 3^{rd}-order process model is applicable with nearly equal performance to a 63^{rd}-order process model, thereby verifying the conjecture that the solution model derived from a simple process model is appropriate to optimize a more detailed process model. The results presented are promising but need to be supported by additional studies, in particular an application to a real process. Furthermore, it would be of interest to investigate the validity of solution models in the presence of other types of uncertainty such as process disturbances.

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