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Time-Optimal Control of Distillation Columns by Iterative Dynamic Programming

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Iterative dynamic programming employing randomly chose candidates for admissible control is applied to minimization of distillation startup time. The solution of this high dimensional problem was facilitated mainly due to avoiding of iterative algebraic equation inside a rigorous dynamic distillation model which is less computer time consumer. The control variable is the reflux ratio. Both piecewise constant control and piecewise linear control strategies were investigated. The decrease of the startup time and heat consumption are high, having an important economic significance.

Introduction

Time-optimal control (TOC) is a challenge in engineering: the general problem of reaching a desired final state from a set of given initial condition in minimum time by an adequate control policy occurs very often in chemical engineering, especially in process startup. This transition should be accomplished as fast as possible because the intermediate product has no economic value. In many cases, the value of utilities and time consumed during the startup period are important, and, in fact, they are wasted.

For high-dimensional nonlinear systems, TOC problems are extremely difficult to be solved. Usually, methods based on dynamic programming were limited to systems with low dimensionality. By introduction of iterative dynamic programming (IDP) by Luus (1989), that employs systematic contraction of the search region and thus dispenses with the need for a fine grid, the problems dimensionality can be significantly increased. However, the applications presented in literature were, especially, from the field of chemical reactors, involving a reduced number of state variables. TOC of startup distillation columns involves much more state variables, being a very high-dimensional problem.

Mathematical Formulation of TOC

The continuous dynamic system is described by differential equations

$$\frac{ds_i}{dt} = f_i(s_1, s_2, ..., s_{ns}, u_1, u_2, ...u_{nu}) \qquad i = 1,2,...,ns \tag{1}$$

where s_i are the state variables with initial state $s_i(0)$, i =1,2,…, ns given, and u_i are control variables subject to the bounds:

$$u_{\min_i} \le u_i \le u_{\max_i} \qquad i = 1,2,...,nu \tag{2}$$

a) Picewise constant control

In order to transform the continuous control policy into a piecewise constant control problem, the time interval $0 \le t \le t_f$ is divided into S time stages of variable length

$$v(k) = t_k - t_{k-1} \qquad k = 1,2,...,S \tag{3}$$

where values of control variables are kept constant during each of these time intervals. The reason of variable length stages is to determine switching times accurately.

By introduction (Bojkov and Luus, 1994) of the normalized time variable τ such that $\tau = t/t_f$ with the discrete values $\tau_k = k/S,\ k = 0,1,...,S$ in the transformed time domain, each stage is of equal length $1/S$. The eqs 1 in the time interval $\tau_k \le \tau \le \tau_{k+1}$ become:

$$\frac{ds_i}{d\tau} = v(k)\, S\, f_i\,(s_1, s_2, ..., s_{ns}, u_1, u_2, ..., u_{nu}) \quad i = 1,2,...,ns;\ \ k = 1,2,...,S \tag{4}$$

The TOC problem is to determine the control variables $u_i(\tau_k)$, $i = 1,2,...,nu; k = 1,2,...,S$ and the length of time stages $v(k), k = 1,2,...,S$ such that

$$s_i(t_f) = s_{s_i} \qquad i = 1,2,...,ns \tag{5}$$

where s_{s_i} are the desired final stationary state values, and the final time t_f is minimized.

In order to minimize the final time t_f subject to constraint eqs 5, the penalty performance index was formulated as

$$I = t_f + \omega \frac{\sum_{i=1}^{ns} \left| 1 - \frac{s_i(t_f)}{s_{s_i}} \right|}{ns} \tag{6}$$

where $\omega > 0$ is a penalty coefficient, and the final values of state variables $s_i(t_f), i = 1,2,...ns$ are calculated by integration of eqs 4.

In applications it was used the TOC algorithm proposed by Bojkov and Luus (1994), based on the IDP procedure employing randomly chose candidates for the admissible control given by Bojkov and Luus (1992, 1993).

b) Piecewise linear control

In some cases a continuous control policy is preferred, rather than a policy that requires sudden switching from one level to another.

According with the procedure proposed by Luus (1993) a piecewise linear control policy u_i in the time interval (t_k , t_{k+1}) is given by:

$$u_i(t) = u_i(k) + \left(\frac{u_i(k+1) - u_i(k)}{t_{k+1} - t_k} \right) (t - t_k) \tag{7}$$

where $u_i(k)$ is the value of u_i at t_k and $u_i(k+1)$ is the value of u_i at t_{k+1}. The optimal control problem then is to find $u_i(k)$, $i = 1,2\ldots,nu; k = 0,1,\ldots,S\text{-}1$, such that the performance index in eq 6 is minimized. For the last stage u_i is kept constant at the value $u_i(S\text{-}1)$. By iterative dynamic programming, eq 7 does not introduce any difficulties, since $u_i(k+1)$ is known from the previous stage and all that remains is to find the best value for $u_i(k)$ at the beginning of the interval. In order to provide a continuous control policy, a single point is used for **s**-grid at each time stage. Luus (1993) considered that despite situation where convergence difficulties may result, from the point of view of simplicity it is a good compromise.

Startup Distillation Operational Procedure

Startup of distillation columns is a very challenging control and simulation problem due to both theoretical and practical aspects. A general sequence of actions which forms the basis for different startup procedures was formulated by Ruiz et al (1988).

At the end of several actions all plates has enough liquid holdup so that the liquid can start to fall down the downcomers. The downcomers are sealed and no vapor can go up through them. The liquid composition is the same on all plates, being equal with the feed composition. In the frame of present work these conditions define the initial state from which begins the effective startup transient operating regime procedure. Traditionally, the column is operated at constant values of control parameters (reflux ratio, reboiler heat duty, etc). Usually, these are the prescribed values for the desired stationary regime. In an optimal transient regime procedure the column will be operated at prescribed time-distributed values of control parameters in order to minimize the duration of the transient regime.

To establish the optimal time-distributed values of control parameters besides a TOC algorithm, an adequate dynamic distillation model (DDM) is needed. This model corresponds with the applied formulation of the general eqs 1 and 2.

Dynamic Distillation Model

In a rigorous dynamic distillation model (DDM) at each time stage representing an integration step of differential mass- and energy-balances, the calculation of temperature and vapor composition on the column plates is made by an iterative procedure solving algebraic nonlinear equations. For optimization purposes, due to the computer time reasons, these models are not suitable. The DDM proposed by Woinaroschy (1986a) represents a good compromise between the degree of complexity and correctness. The advantage and originality of the selected model consist in the fact that the iterative algebraic equations are avoided.

The following simplification assumptions are present in this model:

i) The molar vapor holdup is negligible compared to the molar liquid holdup;

ii) Interphase heat transfer is considered much more intense than interphase mass transport; consequently, the liquid and vapor leaving each plate are in thermal equilibrium at the boiling temperature corresponding to the liquid composition;

iii) On each plate the liquid and vapor are perfectly mixed and Murphree plate efficiency is applied;

iv) Entrainment and weeping rates, flooding of the plates, downcomer holdup, and delay time between plates are neglected.

With exception of the fourth assumption, these hypotheses are present in most of rigorous DDM.

For a typical plate in a distillation column, neglecting the molar vapor holdup, with the usual notation for distillation, mass- and energy-balance equations are defined thus:

Component mass balance around plate *j* for component *i*:

$$\frac{d(N_j x_{i,j})}{dt} = L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} - L_j x_{i,j} - V_j y_{i,j} \pm F_{L,j}x_{F,i,j} \pm F_{V,j}y_{F,i,j} \quad (8)$$

Total mass balance around plate *j*:

$$\frac{dN_j}{dt} = L_{j-1} + V_{j+1} - L_j - V_j \pm F_{L,j} \pm F_{V,j} \tag{9}$$

Total energy balance around plate *j*:

$$\frac{d(N_j h_j)}{dt} = L_{j-1}h_{j-1} + V_{j+1}H_{j+1} - L_j h_j - V_j H_j \pm F_{L,j}h_{F,j} \pm F_{V,j}H_{F,j} - q_j \tag{10}$$

By developing of the left side of eq 8 and after substitution of eqs 9 and reordering, the applied form of component mass balance around plate *j* for component *i* is:

$$\frac{dx_{i,j}}{dt} = \frac{1}{N_j}\left[\begin{array}{l} L_{j-1}(x_{i,j-1} - x_{i,j}) + V_{j+1}(y_{i,j+1} - x_{i,j}) \pm F_{L,j}(x_{F,i,j} - x_{i,j}) \\ \pm F_{V,j}(y_{F,i,j} - x_{i,j}) \end{array}\right] \tag{11}$$

The original feature of the model (due to the iterative solving of nonlinear algebraic equations is avoided) consists in the calculation of the temperature on each plate. Starting from the vapor composition constraint on plate *j*:

$$\sum_{i=1}^{m} \frac{\gamma_{i,j}P_{i,j}}{p_j} x_{ij} = 1 \tag{12}$$

by differentiation versus time of this equation, making several substitutions according with corresponding expressions of the variables, and some other differentiations versus time, an original equation for dynamic calculation of temperature on plate *j* results:

$$\frac{dT_j}{dt} = -\frac{\sum_{i=1}^{m} \frac{\gamma_{i,j}P_{i,j}}{p_j}\left(1 + \frac{x_{i,j}}{\gamma_{i,j}}\frac{d\gamma_{i,j}}{dx_{i,j}}\right)\frac{dx_{i,j}}{dt}}{\sum_{i=1}^{m} \frac{x_{i,j}\gamma_{i,j}}{p_j}\frac{dP_{i,j}}{dT_j}} \tag{13}$$

The core of the model consists in the system of ordinary differential equations 9, 11, and 13, that represent the particularization of the general continuous dynamic system (eq 1). The state variables are N_j, j=1,2..n; $x_{i,j}$, i=1,2..m-1, j=1,2..n; and T_j, j=1,2..n. The reflux ratio can be assigned as control variable **u**.

The variation of total pressure during each time integration step is much more small than the variations of composition and temperature. In order to simplify the procedure, the pressure p_j on the tray *j* is considered constant along the time integration step, but it will be recomputed at the beginning of each new time step:

$$p_j = p_{j+1} - \Delta p_j \tag{14}$$

where the tray pressure drop Δp_j is calculated on the base of hydraulic correlations, specific for the plate type.

Vapor flow rate V_j is obtained from total energy balance (eq 10) and the vapor composition is calculated according to Murphree efficiency. Liquid flow rate L_j is computed on the base of Francis' correlation for the corresponding plate weir. The equilibrium, thermodynamic data, and other physical properties correlations are selected in function of the mixture nature.

The system of differential equations was numerically integrated by fourth order Runge-Kutta-Gill method. Due to the strong nonlinearity of eq 13, a small initial integration step must be used, respectively 2 s. The corresponding increasing of the computer time due to the small value of the integration step is justified by avoiding of

iterative algebraic equations which are higher computer time consumer. This DDM was favorably certified by several theoretical and experimental tests (Woinaroschy, 1986b).

Application

A mixture of four components (60% benzene, 20% toluene, 10% ethylbenzene and 10% o-xylene) is distillated in an industrial scale sieve plates column (30 plates, 3.5 m diameter, lateral downcomers).

The vapor pressures $P_{i,j}$ of components were calculated on the base of Antoine equation.

The TOC algorithm was applied for S=5 time stages, in order to establish the optimal reflux control, for piecewise constant case, and for piecewise linear case (Figure 1). The temperature evolutions in time, on plate 30 (bottom plate), are shown in Figure 2. The grid points number for **s**-grid was 5 for piecewise constant case, and one for piecewise linear case, 9 for **u**-grid, and 9 for ***v***-grid. The region contraction factor was set at 0.8, and the total number of IDP iterations was 10.

The corresponding values of start-up time are: 135 min. for traditional operating procedure (with constant reflux ratio 2), 59 min. for piecewise constant control of reflux ratio, and 48 min. for piecewise linear control of reflux ratio (2.29 and, respectively, 2.81 times lower in comparison with traditional operating procedure). The corresponding heat consumption is reduced from 2815 kWh for traditonal operating procedure to 1230 kWh and, respectively, 1001 kWh.

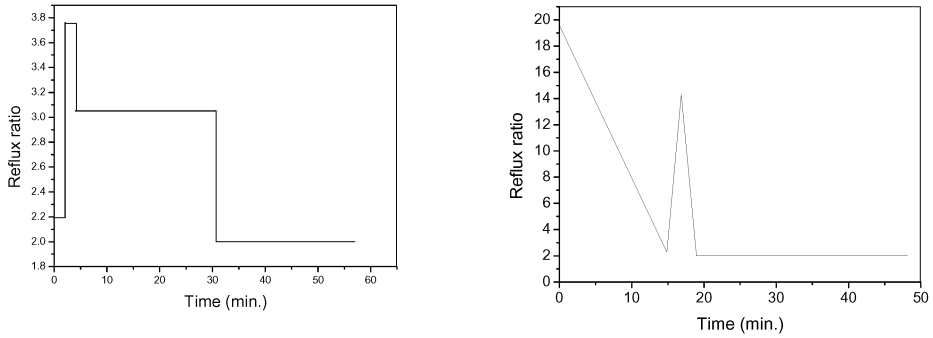

Figure 1. Optimal reflux control for piecewise constant and for piecewise linear cases

Discussion

The selected value for the number of time stages S=5 seems to be too small. A higher value of this number increases exponentially the CPU time without a substantial improving of the performance index. This fact is argued by several references examples (Luus, 1989; Luus and Galli, 1991).

The improvement obtained by TOC of startup distillation in comparison with a traditional startup procedure seems to be artificially amplified. But this traditional startup procedure is frequently used. Due to bang-bang control (especially in the case of piecewise constant), the practical implementation of the optimal policies obtained here can lead to some hydrodynamic problems (flooding, weeping, liquid entrainment, etc). Therefore, it is useful to test these control policies by simulations, using a DDM with

more detailed plate hydraulics. In this way, some sub-optimal control policies, avoiding wrong hydrodynamic regimes, can be identified by suitable corrections.

The procedure used here was also applied with very promising results for azeotropic mixtures, for reboiler heat duty control, and for combination of reflux and reboiler heat duty control.

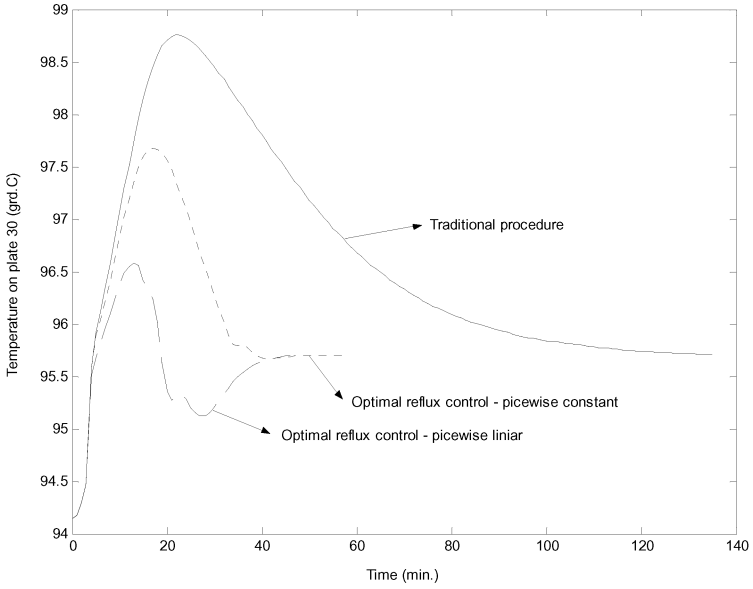

Figure 2. Temperature evolutions in time on plate 30

Conclusions

It was proved the ability of IDP to solve high dimensional TOC problems, involving complex models. Optimal control policies for startup distillation columns were obtained on the base of a DDM representing a good compromise between correctness and complexity. This result was possible mainly due to the transformation of the differential algebraic equations model into an ordinary differential equations model, which is less computer time consumer. The decrease of the startup time and heat consumption were high, having an important economic significance.

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