Unified Approach to Solving Optimal Design-Control Problems in Batch Distillation

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This article presents a unified approach to simultaneous solution of optimization and optimal control problems in batch distillation, operating under different modes of operation: variable, constant, or optimal reflux. The simplified, computationally efficient short-cut method and a novel algorithm to solve the optimal control problems in batch distillation is the basis of this unified approach. The short-cut method identifies the feasible region of operation essential for optimization and optimal control problems, and provides analytical partial derivatives of the model parameters crucial to the solution.

The new algorithm for the solution of optimal control problems is a combination of the maximum principle and NLP optimization techniques. It circumvents the problems associated with the maximum principle approach (iterative solution of a two-point boundary value problem, unbounded control variables, and inability to handle the simultaneous optimization and optimal control problem), and the coupled ODE discretization-NLP optimization scheme for nonlinear models (higher system nonlinearities, multiplicity of solutions, sensitivity of convergence to initial guesses). This algorithm reduces the dimensionality of the problem, and the nature of the algorithm allows a common platform to optimal solutions of different operating conditions. This article also shows that different categories of the optimal control problems in batch distillation essentially involve the solution of the maximum distillate problem.

Introduction

The two well-known methods of operating batch columns are variable reflux and constant product composition of the key component, and constant reflux and variable product composition. The optimal control policy is essentially a trade-off between the two methods and is based on the availability to yield most profitable operation. Literature on optimization of batch column is focused mostly on the solution of optimal control problems, which includes optimizing the indices of performance like maximum distillate, minimum time, and maximum profit. Design optimization of batch columns for constant and variable reflux policies for single and multifraction operation is considered in our earlier work (Diwekar et al., 1989). This work is based on the simplified, computationally efficient short-cut method proposed by Diwekar and Madhavan (Diwekar, 1988; Diwekar and Madhavan, 1991). Recently, Logsdon et al. (1990) have also solved the problem of simultaneous optimization of design and operation of batch columns using the short-cut method, collocation approach, and nonlinear programming (NLP) techniques, with the optimal control policy problem embedded in the overall problem.

Although optimal control policy falls between the two conventional policies, each optimal control problem with different objective functions is treated separately in the literature. This is because of the complexity of the problem formulation and large computational efforts associated with the solution of the optimal control problem. The commonly used methods for solving optimal control problems include Pontryagin's maximum principle and dynamic programming, and use of nonlinear programming algorithms with ODE discretization by collocation. For continuous optimization problems the maximum principle is preferable to dynamic programming, because the application of dynamic programming leads to a set of partial differential equations. The maximum principle necessitates repeated numerical solutions of two-point boundary value problems, thereby making it computationally expensive. Furthermore, it cannot handle bounds on the control variables easily. On the other hand, for nonlinear systems the discretization approach adds nonlinearities to the system (as the number of nonlinear equations are increased), requires good initializations, and may result in multiple solutions.

To circumvent the problems associated with maximum principle (two-point boundary value problem solution and unbounded control variables), the collocation discretization and use of NLP optimization techniques (increased dimensionality), a novel approach to the solution of optimal control problems in batch distillation is presented in this article. The approach is a combination of maximum principle and NLP optimization techniques, and can handle bounds of the control variables. Besides, this algorithm also reduces the dimensionality of the problem and reduces computational efforts. For batch distillation, the use of short-cut method reduces the computational time further.

Apart from the computational efficiency, lower memory requirement, and the algebraic-equation-oriented form (the number of equations is independent of the number of plates and the design variable, N, the number of plates, is not an integer) of the short-cut method, it is also useful in analyzing the optimization problem in a qualitative way. This property is extremely handy in identifying proper bounds for feasible operation. The algebraic nature of the short-cut provides analytical partial derivatives needed to solve the optimal control problem. Based on the short-cut method and the new approach to optimal control solution, this article presents a unified approach for solving optimal design-control problems in multicomponent batch distillation operating under constant reflux, variable reflux, or optimal reflux policy.

It is also shown that the optimal control problems in batch distillation, which are categorized as one of maximum distillate, minimum time, or optimal profit, are not different from each other but essentially involve the solution of the maximum distillate problem.

Previous Work

Batch distillation optimization problems reported in the literature are mostly for the optimal operation of the column with a fixed column design, popularly referred to as optimal control problems. These problems can be classified as:

- *Maximum Distillate Problem.* To maximize the amount of distillate of a specified concentration for a specified time (Converse and Gross, 1963; Keith and Brunet, 1971; Murty et al., 1980; Diwekar et al., 1987; Logsdon et al., 1990; Farhat et al., 1990).
- *Minimum Time Problem.* To minimize the batch time needed to produce a prescribed amount of distillate of a specified concentration (Coward, 1967a,b; Robinson, 1969; Mayur and Jackson, 1971; Egly et al., 1979; Hansen and Jorgensen, 1986; Mujtaba and Macchietto, 1988).
- *Maximum Profit Problem.* To maximize a profit function for a specified concentration of distillate (Kerkhof and Vissers, 1978; Logsdon et al., 1990).

Converse and Gross (1963) first reported the maximum distillate problem for binary batch distillation columns. They used Pontryagin's maximum principle, dynamic programming, and calculus of variation. Diwekar et al. (1987) extended the model for multicomponent systems and used the short-cut method for calculation of the optimal reflux policy. Recently, Logsdon et al. (1990) used finite element collocation and NLP techniques to solve the same problem using the short-cut model. The objective function used by Farhat et al. (1990) can be categorized as a maximum distillate problem, although their aim was to maximize production of specified cuts in the multifraction operation. They considered batch time for each cut also as decision variables. They used linear and exponential approximations to the optimal profiles and applied NLP optimization techniques to obtain the solution.

Early approaches to minimum time problem involved solution of two-point boundary value problems (Coward, 1967a,b; Robinson, 1969; Mayur and Jackson, 1971; Egly et al., 1979; Hansen and Jorgensen, 1986). Mujtaba and Macchietto (1988) used piecewise constant reflux policy and used sequential quadratic programming (SQP) NLP optimizer to solve the problem.

Kerkhof and Vissers (1978) applied the maximum principle to obtain the solution to the maximum profit problem. Logsdon et al. (1990) used ODE discretization and NLP optimization to solve the maximum profit problem formulated by Kerkhof and Vissers, and also extended the profit function to consider the effect of the vapor boilup rate and number of plates.

Literature on optimal design of batch distillation for performing specified operation using constant reflux or variable reflux policy is very limited (Houtman and Hussain, 1956; Robinson and Goldman, 1969; Diwekar et al., 1989; Al-Tuwain and Luyben, 1991).

Optimization involving both differential and algebraic equation models (DAOP) has been the focus of attention in recent literature. Most of the literature in this area concentrates on discretization of ODEs using collocation approach (Cuthrell and Biegler, 1987; Logsdon et al., 1990) or approximating the control profile by polynomials (Akgiray and Heydeweiller, 1990; Farhat et al., 1990), and applying NLP methods to solve the problem. For nonlinear models, the combination of collocation techniques and NLP optimization increases nonlinearities in the system, thereby increasing the possibility of multiple solutions and requiring good initial guesses. On the other hand, the polynomial approximation methods depend on the crucial decision of choosing the right type and order of polynomial for the control profile approximation.

Optimal Control Problem

The differential algebraic optimization problem (DAOP) in general can be stated as follows:

$$\underset{\theta_t,\ \overline{\mu}}{\text{Optimize}}\ J=j\left[\overline{x}_T+\int_0^T k(\overline{x}_t,\ \theta_t,\ \overline{\mu})dt\right] \tag{1}$$

subject to

$$\frac{d\overline{x}_t}{dt}=f(\overline{x}_t,\ \theta_t,\ \overline{\mu}) \tag{2}$$

$$h(\overline{x}_t,\ \theta_t,\ \overline{\mu})=0 \tag{3}$$

$$g(\overline{x}_t,\ \theta_t,\ \overline{\mu})\leq 0 \tag{4}$$

$$\overline{x}_0=\overline{x}_{\text{initial}}$$

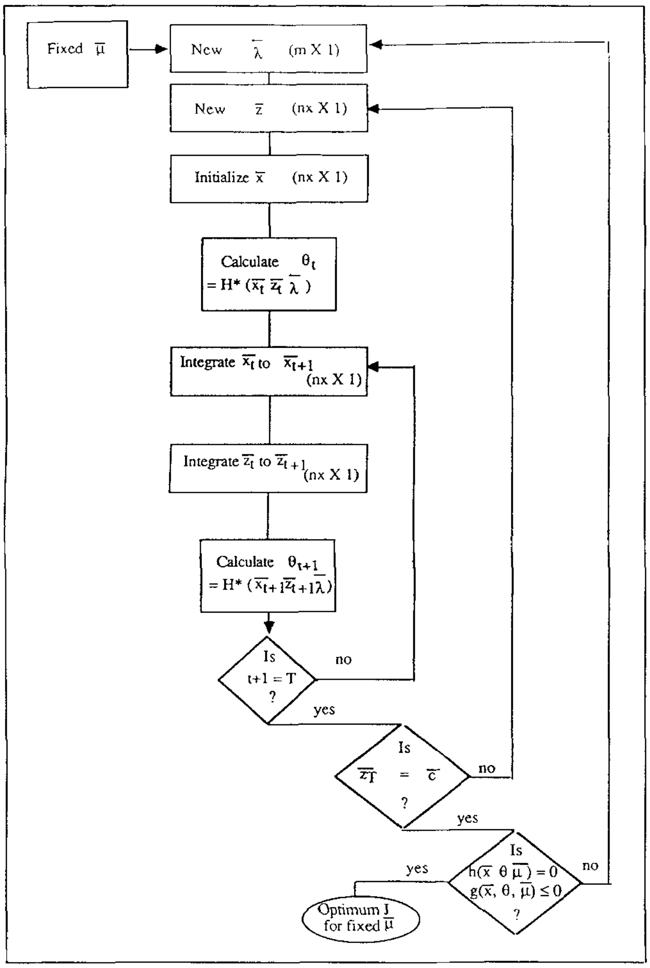

Figure 1. Solution using the maximum principle.

$$\theta(L) \leq \theta_t \leq \theta(U)$$

$$\bar{\mu}(L) \leq \bar{\mu} \leq \bar{\mu}(U)$$

where J is the objective function given by Eq. 1, $\bar{x}_t$ is the state vector ($nx \times 1$ dimensional) at any time t, θ_t is the control vector, and $\bar{\mu}$ is the vector of the scalar variables. Equations 3 and 4 represent the equality (m_1 constraints) and inequality constraints (m_2 constraints including the bounds on the state variables), respectively (total m constraints). $\theta(L)$ and $\bar{\mu}(L)$ represent the lower bounds on the control variables θ_t and the scalar variable μ, respectively, and $\theta(U)$, $\bar{\mu}(U)$ are the upper bounds for the same.

In the absence of the scalar variable vector $\bar{\mu}$, the DAOP is equivalent to the optimal control problem. The most popular method for solving the optimal control problem is Pontryagin's maximum principle method. Recent advances in NLP optimization techniques have provided the researchers with a new tool. Discretization of ODEs to algebraic equations, followed by NLP optimization problem, seems to be the current trend in the optimization literature.

In the following subsections, these two approaches for the solution of the above DAOP are compared. A new algorithm, which tries to overcome the drawbacks of the maximum principle and the ODE discretization followed by NLP optimization, is presented for the solution of optimal control problems in batch distillation. Optimal control problems in batch distillation for various categories of objective functions are also analyzed.

Maximum Principle

The maximum principle was proposed first by Pontryagin and coworkers (Boltyanski et al., 1956; Pontryagin, 1956, 1957). Since then, it has been widely used to solve a variety of optimal control problems. Unfortunately the maximum principle can be used to solve the optimal control problem for a fixed scalar variable vector ($\bar{\mu}$) only, not the complete DAOP described in the previous section. Figure 1 shows the solution to the DAOP for a fixed $\bar{\mu}$ based on the formulation given below.

$$\underset{\theta_t}{\text{Optimize}}\ J = j\left[\bar{x}_T + \int_0^T k(\bar{x}_t, \theta_t, \bar{\mu})dt\right] = \bar{c}^T\bar{x}_T = \sum_{i=1}^{nx} c^i x_T^i \tag{5}$$

subject to

$$\frac{d\bar{x}_t}{dt} = f(\bar{x}_t, \theta_t, \bar{\mu}) \tag{6}$$

$$h(\bar{x}_t, \theta_t, \bar{\mu}) = 0 \tag{7}$$

$$g(\bar{x}_t, \theta_t, \bar{\mu}) \leq 0 \tag{8}$$

$$\bar{x}_0 = \bar{x}_{\text{initial}}$$

$$\theta(L) \leq \theta_t \leq \theta(U)$$

The righthand side of Eq. 5 represents the *linear objective function in terms of the final values* of $\bar{x}$ and values of $\bar{c}$, where $\bar{c}$ represents the vector of constants. Using the Lagrangian formulation for the above problem and removing the bounds $\theta(L)$ and $\theta(U)$ on the control variable vector θ_t, since the maximum principle cannot easily handle the bounds on the control variable (Cuthrell and Biegler, 1987; Akgiray and Heydeweiller, 1990), one obtains:

$$\underset{\theta_t}{\text{Optimize}}\ J^* = \bar{c}^T\bar{x}_T + \bar{\lambda}_1^T[h(\bar{x}_t, \theta_t, \bar{\mu})] + \bar{\lambda}_2^T[g(\bar{x}_t, \theta_t, \bar{\mu})] \tag{9}$$

subject to

$$\frac{d\bar{x}_t}{dt} = f(\bar{x}_t, \theta_t, \bar{\mu}) \tag{10}$$

$$\bar{x}_0 = \bar{x}_{\text{initial}}$$

where

$$\bar{\lambda}^T = [\bar{\lambda}_1^T, \bar{\lambda}_2^T]$$

Application of the maximum principle to the above problem involves addition of nx adjoint variables z_t (one adjoint variable

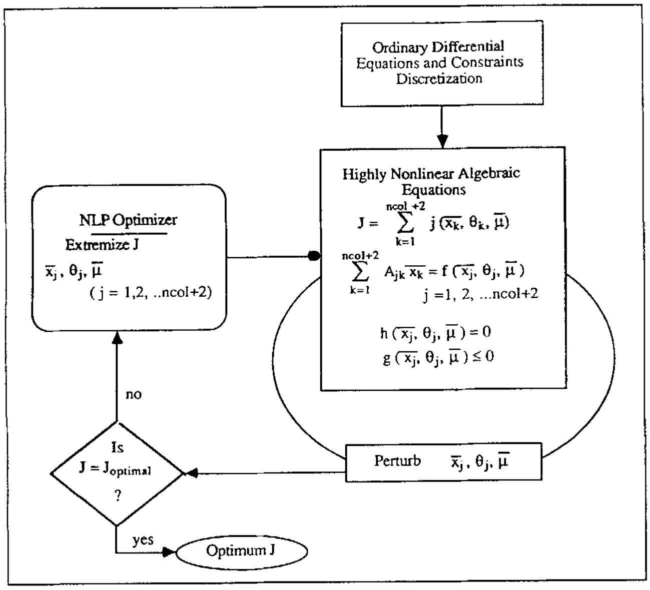

Figure 2. Solution using ODE discretization and NLP optimization.

per state variable), nx adjoint equations, and a Hamiltonian that satisfies the following relations:

$$H(\bar{z}_t, \bar{x}_t, \theta_t) = \bar{z}_t^T f(\bar{x}_t, \theta_t) = \sum_{i=1}^{nx} z_t^i f^i(\bar{x}_t, \theta_t) \tag{11}$$

$$\frac{dz_t^i}{dt} = -\sum_{j=1}^{n} z_t^j \frac{\partial f^j}{\partial x_t^i} \tag{12}$$

$$\bar{z}_0 = \bar{c}$$

The optimal decision vector θ_t can be obtained by extremizing the Hamiltonian given by Eq. 11, and θ_t can then be expressed as:

$$\theta_t = H^*(\bar{x}_t, \bar{z}_t, \bar{\lambda}) \tag{13}$$

Figure 1 represents the control vector iteration solution procedure for the optimal control problem using the maximum principle. For the initial values of $\bar{\lambda}$ and the vector $\bar{z}$, the vector $\bar{x}$ is initialized and θ_0 (θ_t at $t=0$) is obtained from Eq. 13. Equations 10 and 12 are integrated to get $\bar{x}$ and $\bar{z}$, and θ_{t+1} is calculated using the Eq. 13. The integration of Eqs. 10 and 12, and calculation of θ_{t+1} continue until the final time T is reached. At this stage, the final value of the vector $\bar{z}_T$ is compared with $\bar{c}$. The procedure is repeated until the vectors $\bar{z}$ and $\bar{c}$ are equal. The calculation control is then transferred to the final loop for the evaluation of $\bar{\lambda}$. The final loop converges when all the constraints are satisfied.

The procedure in Figure 1 shows that this approach is computationally intensive as it needs an iterative solution of the two-point boundary value problem. Beside the drawbacks associated with the computational intensity, the method cannot handle the bounds on the control variables very easily and is restricted to the solution of the optimal control problem for fixed scalar variables only.

Orthogonal collocation and nonlinear programming optimization

This approach involves discretization of the state variables in terms of polynomial approximation using the orthogonal collocation technique. The discretization converts the set of differential equations to a set of nonlinear algebraic equations, which can then be solved using NLP optimization techniques.

Discretizing the state and control variables in terms of Lagrange polynomial $[l_i(t)]$ results in the following:

$$\bar{x}_t = \sum_{i=1}^{n\,\mathrm{col}+2} l_i(t)\bar{x}_i;\ \theta_t = \sum_{i=1}^{n\,\mathrm{col}+2} l_i(t)\theta_i \tag{14}$$

$$\frac{d\bar{x}_t}{dt} = \sum_{i=1}^{n\,\mathrm{col}+2} A_{ki}\bar{x}_i \tag{15}$$

where A_{ki}'s are the coefficients arising from differentiating the Lagrange polynomials:

Substituting the values of $\bar{x}_i$, θ_i and $(d\bar{x}_i/dt)$ from the above equations, the DAOP reduces to:

$$\underset{\bar{\mu},\, \bar{x}_j,\, \theta_j,\, j=1,\,\ldots,\, n\mathrm{col}+2}{\text{Optimize}} \quad J = j\left[\sum_{i=1}^{n\mathrm{col}+2} l_i(T)x_i + \sum_{i=1}^{n\mathrm{col}+2} w_i k(\bar{x}_i, \theta_i, \bar{\mu})\right] \tag{16}$$

subject to

$$\sum_{i=1}^{n\mathrm{col}+2} A_{ji}\bar{x}_i = f(\bar{x}_j, \theta_j, \bar{\mu});\ j=1,\ \ldots,\ n\mathrm{col}+2 \tag{17}$$

$$h(\bar{x}_j, \theta_j, \bar{\mu}) = 0,\ j=1,\ \ldots,\ n\mathrm{col}+2 \tag{18}$$

$$g(\bar{x}_j, \theta_j, \bar{\mu}) \le 0,\ j=1,\ \ldots,\ n\mathrm{col}+2 \tag{19}$$

$$\bar{x}_0 = \bar{x}_{\mathrm{initial}}$$

$$\theta(L) \le \theta_i \le \theta(U),\ i=1,\ \ldots,\ n\mathrm{col}+2$$

$$\bar{\mu}(L) \le \bar{\mu} \le \bar{\mu}(U)$$

The solution strategy of this method is presented in Figure 2, which shows that discretization increases the dimensionality of the system. For nonlinear systems, this is equivalent to increasing nonlinearities, which may lead to multiple solutions, and thus good initial values are necessary to achieve convergence.

New algorithm

The maximum principle discussed earlier is a powerful tool for solving optimal control problems. However, simultaneous solution of optimization and optimal control problems is not possible using the maximum principle. Furthermore, solution of the two-point boundary value problem and the additional adjoint equations with the iterative constraint satisfaction can be computationally very expensive. Additionally, the nature

Table 1. Time Implicit Model Equations for the Short-Cut Method

Differential Material Balance Equation
$x_{B_{new}}^{(i)} = x_{B_{old}}^{(i)} + \frac{\Delta x_B^{(1)}(x_D^{(i)} - x_B^{(i)})_{old}}{(x_D^{(1)} - x_B^{(1)})_{old}}, \; i=1, 2, \ldots, n$
Hengestebeck-Geddes' Equation
$x_D^{(i)} = \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x_D^{(1)}}{x_B^{(1)}} x_B^{(i)}, \; i=2, 3, \ldots, n$
Summation of Fractions
$\sum_{i=1}^{n} x_D^{(i)} = 1$
$x_D^{(1)}$ estimation
$x_D^{(1)} = \frac{1}{\sum_{i=1}^{n} \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x_B^{(i)}}{x_B^{(1)}}}$
Fenske Equation
$N_{min} \approx C_1$
Underwood Equations
$\sum_{i=1}^{n} \frac{\alpha_i x_B^{(i)}}{\alpha_i - \phi} = 0; \; R_{min\,u} + 1 = \sum_{i=1}^{n} \frac{\alpha_i x_D^{(i)}}{\alpha_i - \phi}$
Gilliland Correlation
C_1 Estimation
$R_{min\,g} = F(N, N_{min}, R)$
$\frac{R_{min\,g}}{R} - \frac{R_{min\,u}}{R} = 0$

of the problem does not allow bounds on the variables. On the other hand, the orthogonal collocation discretization and NLP optimization method can solve the overall optimization problem but involves solution of higher dimensional system of equations.

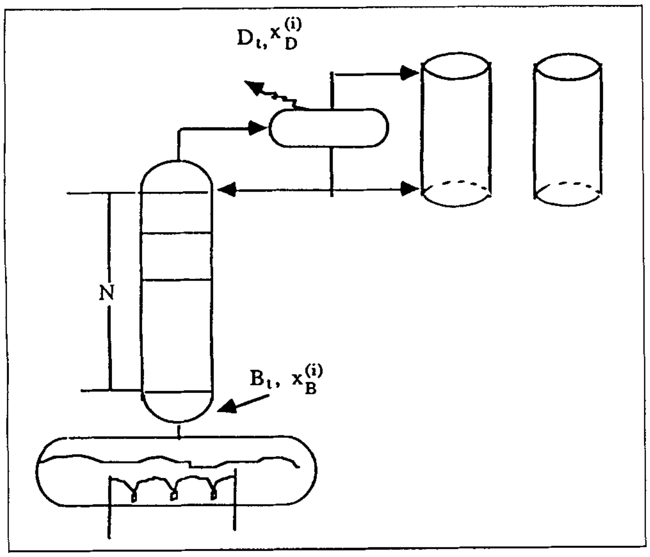

Figure 3. Batch distillation column.

A new approach to optimal control problems in batch distillation proposed here combines the maximum principle and NLP techniques. The number of adjoint variables is reduced by introducing quasi-steady-state approximations (for example, the time implicit differential material balance in Table 1) to some of the state variables, thereby reducing the number of adjoint equations. If the number of equality constraints (other than the system model) and the number of reduced adjoint variables are equal, as in the case of batch distillation, where one adjoint variable z and one equality constraint are specified in terms of product purity (Eq. 29), then neither the Lagrangian formulation of the objective function (Eq. 9) nor the final boundary conditions of the adjoint variables ($\bar{z}_0 = \bar{c}$) are used in the solution. Instead, the final boundary conditions of the adjoint variables are automatically imposed when the equality constraints are satisfied. Minimizing the Hamiltonian provides the functional correlation for the control vectors (Eq. 23). In short, the new algorithm involves solution of the NLP optimization problem for the scalar variables $\bar{\mu}$ subject to the original model for the state variables, the adjoint equations (Eq. 22), correlation for the control variables (Eq. 23), and constraints that implicitly relate to the initial values of the adjoint variables (Eq. 24). This algorithm reduces the dimensionality of the problem and avoids the solution of two-point boundary value problem. The following sections show that for the batch distillation problem bounds could be imposed on the control vector by virtue of the nature of the formulation.

The formulation of the DAOP using the new algorithm results in:

$$\underset{\bar{\mu}}{\text{Optimize}}\, J = j\left[\bar{x}_T + \int_0^T k(\bar{x}_t, \theta_t, \bar{\mu})dt\right] \tag{20}$$

subject to

$$\frac{d\bar{x}_t}{dt} = f(\bar{x}_t, \theta_t, \bar{\mu}) \tag{21}$$

$$\frac{d\bar{z}_t}{dt} = f^*(\bar{x}_t, \theta_t, \bar{\mu}) \tag{22}$$

$$\theta_t = H^*(\bar{z}_t, \bar{x}_t) \tag{23}$$

$$\bar{z}_0 = h^*(h(\bar{x}_t, \theta_t, \bar{\mu})) \tag{24}$$

$$g(\bar{x}_t, \theta_t, \bar{\mu}) \leq 0 \tag{25}$$

$$\bar{x}_0 = \bar{x}_{initial}$$

$$\bar{\mu}(L) \leq \bar{\mu} \leq \bar{\mu}(U)$$

$$\theta(L) \leq \theta_t \leq \theta(U)$$

Maximum distillate problem in batch distillation

For the system in Figure 3, which assumes a constant boilup rate and no holdup conditions, an overall differential material balance equation over time dt can be given as:

$$\frac{dx_t^1}{dt}=\frac{dB_t}{dt}=\frac{-V}{R_t+1},\ x_0^1=B_0=F, \tag{26}$$

where F is the feed, which is the initial condition to x_t^1. A material balance for the key component 1 over the differential time dt is:

$$\frac{dx_t^2}{dt}=\frac{V}{R_t+1}\frac{(x_B^{(1)}-x_D^{(1)})}{B_t},\ x_0^2=x_F^{(1)} \tag{27}$$

where

x_t^1 = state variable at time t representing quantity of charge remaining in the still, B_t, mol
x_t^2 = state variable representing the composition of the key component in the still at time t, $x_B^{(1)}$, mol fraction
R_t = control variable vector, reflux ratio, function of time
V = molar vapor boilup rate, mol·h^{-1}
$x_D^{(1)}$ = overhead or distillate composition for key component 1, mol fraction
t = batch time, h

Other state variables are assumed to be in a quasi-steady state and may be obtained using the time-implicit form of short-cut method equations in Table 1. The quasi-steady-state approximation reduces the dimensionality of the problem, since the number of adjoint variables and equations do not increase with the number of components. So the maximum distillate problem can be stated as:

$$\underset{R_t}{\text{Maximize}}\ J=\int_0^T D_t\,dt=\int_0^T \frac{V}{R_t+1}dt, \tag{28}$$

subject to the following purity constraint on the distillate:

$$x_{Dave}=\frac{\int_0^T x_D^{(1)}\frac{V}{R_t+1}dt}{\int_0^T \frac{V}{R_t+1}dt}=x_D^* \tag{29}$$

The problem can be written as:

$$\underset{R_t}{\text{Maximize}}\ -x_T^1, \tag{30}$$

subject to Eqs. 26 and 27, and the time-implicit model in Table 1.

The time-implicit model provides correlations between the model parameters and the state variables. At any time instance, there is change in the still composition of the key component (state variable x_t^2), resulting in changes in the still composition of all the other components calculated by the differential material balance equations (Table 1). Hengestebeck-Geddes' equation relates the distillate composition to the new still composition in terms of constant C_1. Constant C_1 in Hengestebeck-Geddes' equation is equivalent to the minimum number of plates $N_{\min}$ in the Fenske equation. At this stage, C_1 and $x_D^{(1)}$ are the unknowns. Summation of distillate compositions can be used to obtain $x_D^{(1)}$ and the Fenske-Underwood-Gilliland (FUG) equations (Table 1) to obtain C_1.

The Hamiltonian function, which should be maximized is,

$$H_t=-z_t^1\frac{V}{R_t+1}+z_t^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)B_t} \tag{31}$$

and the adjoint equations,

$$\frac{dz_t^1}{dt}=z_t^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)(B_t)^2},\ z_T^1=-1, \tag{32}$$

$$\frac{dz_t^2}{dt}=-z_t^2\frac{V\left(1-\frac{\partial x_D^{(1)}}{\partial x_B^{(1)}}\right)}{(R_t+1)B_t},\ z_T^2=0 \tag{33}$$

Combining the two adjoint variables z^1 and z^2 into one using $z_t=z_t^2/z_t^1$, results in the following adjoint equation:

$$\frac{dz_t}{dt}=-z_t\frac{V\left(1-\frac{\partial x_D^{(1)}}{\partial x_B^{(1)}}\right)}{(R_t+1)B_t}-(z_t)^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)(B_t)^2} \tag{34}$$

The optimality condition on the reflux policy $(dH_t)/(dR_t)=0$, leads to:

$$R_t=\frac{B_t-z_t(x_B^{(1)}-x_D^{(1)})}{z_t\frac{\partial x_D^{(1)}}{\partial R_t}}-1. \tag{35}$$

It should be remembered that this solution (Eq. 35) is obtained by minimizing the Hamiltonian (maximizing the distillate) which does not incorporate the purity constraint (Eq. 29). Hence, use of the final boundary condition ($z_T=0$) provides the limiting solution resulting in all the reboiler charge instantaneously going to the distillate pot ($R=-\infty$) with lowest overall purity. Since in this formulation the purity constraint is imposed external to the Hamiltonian, the final boundary condition ($z_T=0$) is no longer valid.

The short-cut method allows one to obtain the analytical partial derivatives for $(\partial x_D^{(1)})/(\partial R_t)$ and $(\partial x_D^{(1)})/(\partial x_B^{(1)})$ in the above equation.

Minimum time problem in batch distillation

The differential equations for the system shown in Figure 3 can be represented as:

$$\frac{dx_t^1}{dt}=\frac{dB_t}{dt}=\frac{-V}{R_t+1},\ x_0^1=B_0=F,\ x_T^1=B_T, \tag{36}$$

where B_T is the amount remaining in the still at the end of the operation. The material balance for the key component 1 over the differential time dt is:

$$\frac{dx_t^2}{dt}=\frac{V}{R_t+1}\frac{(x_B^{(1)}-x_D^{(1)})}{B_t},\ x_0^2=x_F^{(1)} \tag{37}$$

The other state variables are assumed to be obeying the time implicit model in Table 1 as stated in the maximum distillate problem. For the minimum time problem, however, a new dummy variable t^* is introduced as the third state variable and the relation of t^* with the actual batch time t is given by:

$$\frac{dx_t^3}{dt}=\frac{dt^*}{dt}=1,\ t_0^*=0 \tag{38}$$

The minimum time problem can then be written as:

$$\underset{R_t}{\text{Maximize}}\ J=-\int_0^T dt^*\,dt, \tag{39}$$

subject to the following purity constraint on the distillate.

$$x_{D\text{ave}}=\frac{\int_0^T x_D^{(1)}\frac{V}{R_t+1}dt}{\int_0^T \frac{V}{R_t+1}dt}=x_D^*. \tag{40}$$

Applying the maximum principle, the problem transforms to:

$$\underset{R_t}{\text{Maximize}}\ -x_T^3 \tag{41}$$

subject to Eqs. 36 and 37, and the time implicit model in Table 1.

The Hamiltonian function which should be maximized is:

$$H_t=-z_t^1\frac{V}{R_t+1}+z_t^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)B_t}+z_t^3 \tag{42}$$

and the associated adjoint equations are:

$$\frac{dz_t^1}{dt}=z_t^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)(B_t)^2}, \tag{43}$$

$$\frac{dz_t^2}{dt}=-z_t^2\frac{V\left(1-\frac{\partial x_D^{(1)}}{\partial x_B^{(1)}}\right)}{(R_t+1)B_t},\ z_T^2=0, \tag{44}$$

$$\frac{dz_t^3}{dt}=0,\ z_T^3=-1 \tag{45}$$

Solution of Eq. 45 for z^3 gives:

$$z_t^3=-1 \tag{46}$$

The resulting Hamiltonian function is:

$$H_t=-z_t^1\frac{V}{R_t+1}+z_t^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)B_t}-1 \tag{47}$$

Once again, combining the two adjoint variables into one variable using $z_t=z_t^2/z_t^1$, one obtains the following adjoint equations:

$$\frac{dz_t}{dt}=-z_t\frac{V\left(1-\frac{\partial x_D^{(1)}}{\partial x_B^{(1)}}\right)}{(R_t+1)B_t}-(z_t)^2\frac{V(x_B^{(1)}-x_D^{(1)})}{(R_t+1)(B_t)^2} \tag{48}$$

The optimality condition on the reflux policy $(dH_t)/(dR_t)=0$, leads to:

$$R_t=\frac{B_t-z_t(x_B^{(1)}-x_D^{(1)})}{z_t\frac{\partial x_D^{(1)}}{\partial R_t}}-1, \tag{49}$$

The time optimal problem involves solution of the state variable differential equations (Eqs. 36 and 37) and the adjoint Eq. 48 along with the implicit model in Table 1, and Eq. 49, which relates the control variable to the model parameters and adjoint variables. It can be seen that the time optimal problem involves solution of same set of equations (Eqs. 36, 37, 48, and 49) as that of maximum distillate problem (Eqs. 26, 27, 34 and 35), except that the stopping criterion is different for the two.

Maximum profit problem

Very few researchers have done work in optimizing a profit function for constant reflux, variable reflux, or optimal reflux operating conditions. Kerkhof and Vissers (1978) were the first to use the profit function for maximization and they solved the optimal control problem, their objective function did not include the effect of number of plates and vapor boilup rate. Diwekar et al. (1989) used a different objective function to solve the profit maximization problem for constant and variable reflux conditions. Recently Logsdon et al. (1990) formulated a new profit function and solved the DAOP for optimal design and operation. In the previous section it was shown that the time optimal control problem and maximum distillate problem result in the same solution. In this section it will be shown that the maximum profit problem also involves the solution of the maximum distillate problem.

- Maximization of Profit (Kerkhof and Vissers, 1978):

$$\underset{R_t,\ T}{\text{Maximize}}\ J=\frac{DP_r-B_0C_0}{T+t_s} \tag{50}$$

where

D = amount of product distilled, mol
P_r = sales value of the product
B_0 = amount of feed F, mol
C_0 = cost of feed
T = batch time, h
t_s = setup time for each batch, h

The problem can be converted as:

$$\underset{T}{\text{Maximize}}\ \frac{\left(\underset{R_t}{\text{Maximize}}\ D\right)P_r-B_0C_0}{T+t_s} \tag{51}$$

- Maximization of Profit (Diwekar et al., 1989):

$$\underset{R_t,\,N,\,T,\,V}{\text{Maximize}}\ J=\frac{24(365)DP_r}{T+t_s}-\frac{c_1VN}{G_a}-\frac{c_2V}{G_b}-\frac{24(365)c_3VT}{T+t_s} \tag{52}$$

where c_1, c_2, and c_3 are the cost coefficients and G_a is allowable vapor velocity, and G_b, vapor handling capacity of the equipment.

The objective function may be expressed as a maximum distillate problem as shown below:

$$\underset{N,\,T,\,V}{\text{Maximize}}\ \frac{24(365)\left(\underset{R_t}{\text{Maximize}}\,D\right)P_r}{T+t_s}-\frac{c_1VN}{G_a}-\frac{c_2V}{G_b}-\frac{24(365)c_3VT}{T+t_s} \tag{53}$$

- Maximization of Profit (Logsdon et al., 1990):

$$\underset{R_t,\,T,\,N}{\text{Maximize}}\ J=\frac{DP_r-B_0C_0}{T+t_s}-\frac{K_1V^{0.5}N^{0.8}-K_2V^{0.65}-K_3V}{HRs} \tag{54}$$

where K_1, K_2, and K_3 represent the cost coefficients and HRs represents the hours per year. Converting the problem for application of the new algorithm;

$$\underset{T,\,N}{\text{Maximize}}\left[\frac{\left(\underset{R_t}{\text{Maximize}}\,D\right)P_r-B_0C_0}{T+t_s}-\frac{K_1V^{0.5}N^{0.8}-K_2V^{0.65}-K_3V}{HRs}\right] \tag{55}$$

Overall solution

The solution procedure using the algorithm proposed in this work is shown in Figures 4 and 5. The two levels of optimization are: the NLP optimization at the outer loop with respect to the scalar variables μ, and initial value of $R_t(=R_0)$ and the inner loop involving calculation of the objective function and the purity constraint for fixed values of the scalar variables and R_0. [R_0 is used as the decision variable instead of z_0 as proposed in the new algorithm (Eq. 24), because with this formulation it is easier to put bounds on R_t.]

Given the scalar variables (for example, N and V), and the value of R_0, the inner loop initializes the two state variables, and the short-cut method equations allow for the calculation of the other state variables and model parameters (such as still and distillate composition). The initial value of the adjoint variable is then calculated from the implicit correlation (Eq. 35), thus defining the relationship between the control variable (R_t) with respect to the adjoint variable (z_t) and other model variables. The adjoint equation and state equations are integrated for the next time step and the new R_t is calculated. The integration and calculation of the control variable R_t continue till the specified stopping criterion is met. This stopping criterion in Figure 5 depends on the problem at hand. For maximum profit and maximum distillate problems, the final batch time is used as the stopping criterion and for minimum time problem it is the final amount remaining in the still which marks the end of operation. The values of the objective function and the constraint are calculated at this stage and the control is transferred to the NLP problem, which then computes the new set of scalar variables $\bar{\mu}$ and R_0.

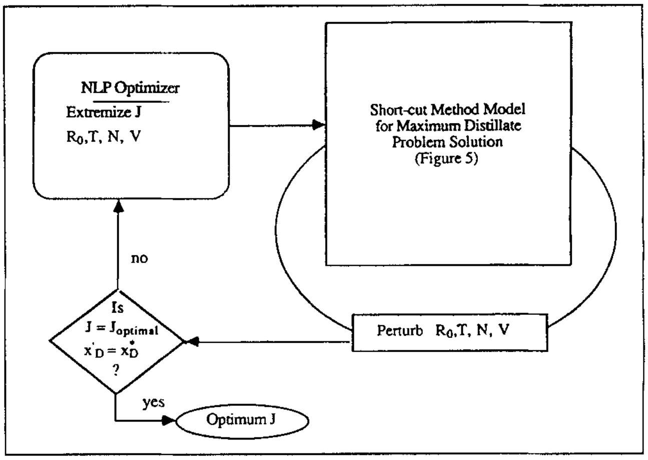

Figure 4. Combining maximum principle and NLP optimization techniques.

Since the variable R_0 is independent of the optimal control problem and it has been observed that the following constraint on R_0 is always valid (Converse and Gross, 1963; Keith and Brunet, 1971; Murty et al., 1980; Diwekar et al., 1987; Logsdon

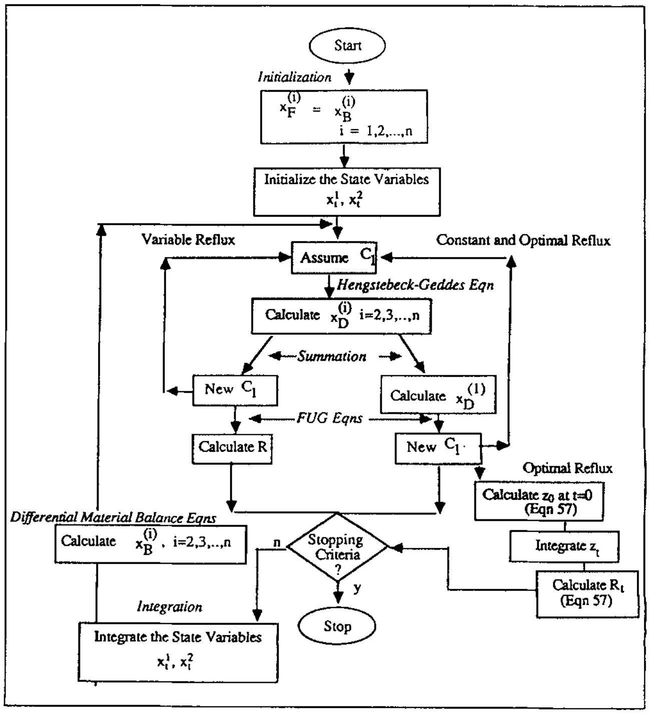

Figure 5. Unified short-cut model for NLP optimization.

Table 2. A Unified Approach Using the Short-Cut Method

	Variable Reflux	Constant Reflux	Optimal Reflux
		Differential Material Balance Equation	
		$x_{B_{\text{new}}}^{(i)}=x_{B_{\text{old}}}^{(i)}+\dfrac{\Delta x_B^{(1)}(x_D^{(i)}-x_B^{(i)})_{\text{old}}}{(x_D^{(1)}-x_B^{(1)})_{\text{old}}},\ i=1,\ 2,\ \ldots,\ n$	
		Hengestebeck-Geddes' Equation	
		$x_D^{(i)}=\left(\dfrac{\alpha_i}{\alpha_1}\right)^{C_1}\dfrac{x_D^{(1)}}{x_B^{(1)}}x_B^{(i)},\ i=2,\ 3,\ \ldots,\ n$	
Unknowns	$R,\ C_1$	$C_1,\ x_D^{(1)}$	$R,\ C_1,\ x_D^{(1)}$
		Summation of Fractions	
		$\sum_{i=1}^{n}x_D^{(i)}=1$	
	C_1 Estimation $\sum_{i=1}^{n}\left(\dfrac{\alpha_i}{\alpha_1}\right)^{C_1}\dfrac{x_D^{(1)}}{x_B^{(1)}}x_B^{(i)}=1$	$x_D^{(1)}$ Estimation $x_D^{(1)}=\dfrac{1}{\sum_{i=1}^{n}\left(\dfrac{\alpha_i}{\alpha_1}\right)^{C_1}\dfrac{x_B^{(i)}}{x_B^{(1)}}}$	
		Fenske Equation	
		$N_{\min}\approx C_1$	
		Underwood Equations	
		$\sum_{i=1}^{n}\dfrac{\alpha_i x_B^{(i)}}{\alpha_i-\phi}=0;\ R_{\min u}+1=\sum_{i=1}^{n}\dfrac{\alpha_i x_D^{(i)}}{\alpha_i-\phi}$	
		Gilliland Correlation	
	R Estimation $R=F(N,\ N_{\min},\ R_{\min u})$	C_1 Estimation $R_{\min g}=F(N,\ N_{\min},\ R)$ $\dfrac{R_{\min g}}{R}-\dfrac{R_{\min u}}{R}=0$	R Estimation $R=F$(Minimum Hamiltonian), Eq. 57

et al., 1990; Coward, 1967a; Robinson, 1969; Mayur and Jackson, 1971; Egly et al., 1979; Hansen and Jorgensen, 1986; Kerkhof and Vissers, 1978),

$$R_0\leq R_t \tag{56}$$

the lower bound $[R(L)]$ may be imposed on the control profile as a lower bound to the decision variable R_0 in the NLP optimization. In fact, it will be shown in the next section that the variable R_0 has an inherent lower bound defined by the purity constraint.

The optimal control profile evaluations stop at the stopping criterion. Alternatively, the upper bound to R_t $[=R(U)]$ can be used as the intermediate stopping criterion for the optimal control problem and the integration of state variable equations continue as in the constant reflux case, with the reflux ratio equal to the upper bound, till the real stopping criteria is encountered.

So, Eqs. 35 and 49 can be written as:

$$\begin{aligned} R_t&=\frac{B_t-z_t(x_B^{(1)}-x_D^{(1)})}{z_t\dfrac{\partial x_D^{(1)}}{\partial R_t}}-1 \quad \text{for} \quad R_t\leq R(U) \\ R_t&=R(U) \quad \text{for} \quad R_t>R(U) \end{aligned} \tag{57}$$

This equation allows one to impose the upper bound on the control profile locally. The successful validation of this strategy is shown in the section on Results and Discussions.

Unified Approach to the Optimization Problems in Batch Distillation

The short-cut method for batch distillation proposed by Diwekar and Madhavan (1991) is based on the assumption that the batch distillation column can be considered as a continuous distillation column with changing feed at any time instant. This approximation enabled the use of continuous distillation theory to batch distillation with some modifications. This model has an algebraic-equation-oriented form, and the different operating conditions (constant reflux and variable reflux) can be simulated using this method. These different operating conditions involve solution of the same set of equations. If the optimal control problem is solved as a maximum distillate problem, then the optimal reflux mode of operation can also be simulated using the same set of equations as those used in the constant reflux and variable reflux cases, with additional equations for calculation of the reflux ratio profiles. Since the model equations are similar, a unified approach to optimization can be proposed. Table 2 gives the modeling equations for all the three modes of operation.

The degrees of freedom analysis presented in our earlier work (Diwekar et al., 1989) resulted in maximum three degrees of freedom for the single fraction case (in the absence of holdup) for both variable reflux and constant reflux operating conditions. It can be seen that the same three degrees of freedom are available for the optimal reflux problem. The optimal decision variables could be initial reflux ratio, R_0 (fixed by the purity constraint as shown in Figures 4 and 5), the stopping criterion T, the number of plates N, and the vapor rate V. To maintain the feasibility of design, appropriate constraints on the variables are to be imposed, especially for the design variables like the number of plates N and the reflux ratio R. The short-cut method helps to identify these bounds on the design parameters. The bounds on the parameters depend on the operating modes. For the variable reflux and the constant reflux condition, the feasible region of operation has been identified using the short-cut method (Diwekar et al., 1989). This new algorithm along with the short-cut method provides for the identification of bounds on the parameters for optimal reflux conditions as well.

For the variable reflux case, the value of $x_D^{(1)}$ $(=x_D^*)$ is specified and the reflux ratio is at its minimum value at the initial conditions. So, the lower bound to R_0 is the value of $R_{\min}$ at the initial conditions (which will need the infinite number of plates for the given separation $x_D^{(1)}=x_D^*$). The upper limit is governed by $N_{\min}$ at the termination criterion. To obtain the upper limit on R, $N_{\min}$ is calculated at the terminal condition and is taken as the limiting value of N. The value of R corresponding to this N to attain the distillate purity specified by x_D^* at the initial condition is the value of $R_{\max}$, the upper bound to R_0.

For both constant reflux and optimal reflux conditions, the initial value of R has a lower bound defined by the specified average distillate composition of the key component x_D^*. The initial distillate composition of the key component (more volatile) is the highest at the beginning and decreases as distillation progresses. If the initial value of R is such that the distillate composition of the key component is less than the specified average, then the goal to attain the specified average purity is impossible to be met for the given number of plates. This criterion provides the lower limit R_{MIN} to the initial R, where R_{MIN} is defined as the value of R required to obtain the distillate composition of the key component $(x_D^{(1)})$ equal to the specified average distillate composition (x_D^*) at the initial conditions for the given N. Similarly, the value of N is also restricted by the lower bound $N_{\min}$ using the same criterion. Here, $N_{\min}$ is the Fenske value of the minimum number of plates for the same value of distillate composition. All the bounds for the three operating modes based on the short-cut method are presented in the tabular form in Table 3.

Figure 4 provides a unified short-cut method model which can be used in conjunction with Figure 5 to solve any single fraction optimization problem. The new approach will be extended to the multifraction case in our future work.

Table 3. Feasible Region for Multicomponent Batch Distillation Columns

Variable Reflux	Constant Reflux	Optimal Reflux
	Final Still Composition	
	$0\le x_{B_{\text{final}}}^{(1)}\le x_D^{(1)}$	
	Distillate Composition	
	$x_B^{(1)}\le x_D^{(1)}\le 1$	
	Reflux Ratio	
$1\le \frac{R_{\text{initial}}}{R_{\min}}\le\frac{R_{\max}}{R_{\min}}$	$1\le\frac{R}{R_{\text{MIN}}}\le\infty$	
	Number of Plates	
$N_{\min f}\le N$	$N_{\min}\le N$	

Results and Discussions

The algorithm proposed in this work was applied to different optimal control problems in the batch distillation literature. The test problems include consideration of different objective functions and operating conditions. The aim of the exercise was to compare the results obtained by using different techniques with the new algorithm results. Since most of the examples in the literature on the optimal control problem are restricted to ideal systems and zero holdup conditions, the test examples are also limited to ideal systems and columns with negligible holdup effects. The algorithm, however, can be extended to include holdup consideration using the modified short-cut model (Diwekar and Madhavan, 1991). For nonideal conditions, the short-cut model optimal control profiles can be used as a preliminary solution. With the recent extension of the short-cut method for binary and ternary azeotropic systems (Diwekar, 1991; Kalagnanam and Diwekar, 1992) the optimal control algorithm can be applied to azeotropic systems.

Comparisons of solution of four different cases of optimal control problems with the profiles obtained by the unified approach and the present algorithm proposed in this article are shown in Figure 6. The types of problem considered include maximum distillate, minimum time, maximum profit, and maximum profit with bounded control profile.

Figure 6a shows the control profiles obtained as a solution to the maximum distillate problem for a quaternary system reported by Diwekar et al. (1987), and Figure 6b the minimum time problem from Coward (1967a). The maximum profit problem with (Figure 6d) and without (Figure 6c) bounds on the control variables is taken from Logsdon et al. (1990). The input data for the problems along with the specifications are shown in Table 4. The profiles obtained by the new algorithm agree very well with the literature results.

For the maximum distillate problem, the reported solution

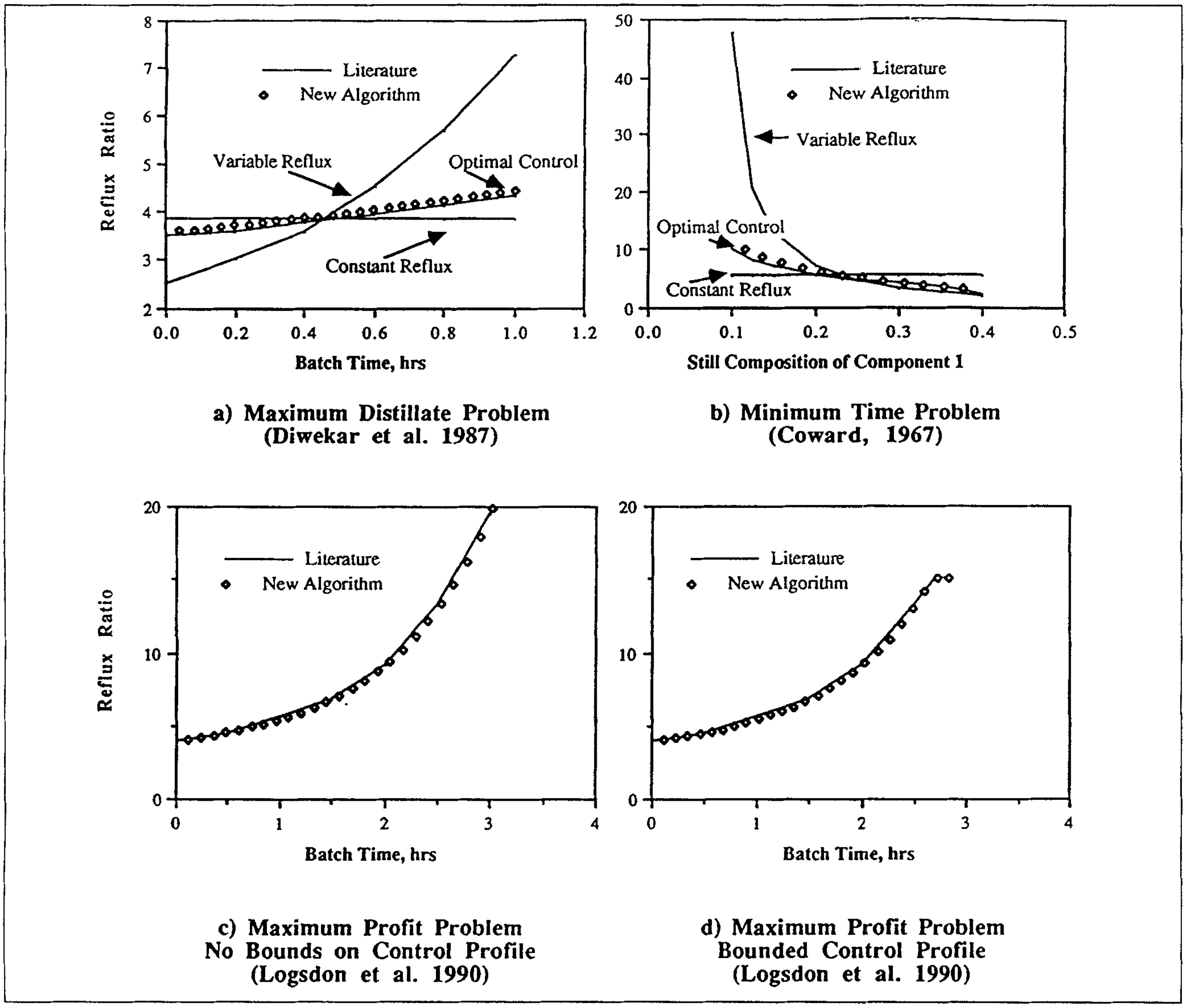

Figure 6. Solution for different DAOPs in batch distillation.

procedure involved iterations on λ and the complete reflux profile R_t, while the new algorithm involved solution of nonlinear algebraic equations with a single iterative variable R_0. Although the CPU time required depends on the initial values of λ and R_t for the two-point boundary value maximum principle, on an average the new algorithm was found to be about 20 times faster than the two-point boundary value formulation for the example shown in Figure 6a.

The time optimal problem shown in Figure 6b was solved using the Fibonacci search technique and the plate-to-plate model. The new algorithm used the same maximum distillate problem to solve this time optimal problem and involved solution of algebraic equations resulting from the short-cut model.

The simultaneous optimal design and operation problem from Logsdon et al. (1990) was solved using the collocation discretization and NLP optimization. Logsdon et al. (1990) have also used the short-cut model for batch distillation to solve this problem. The number of variables used as decision variables in their formulation includes the 12 discretized state variables (associated with each x_i), 12 decision variables for the control vector θ, the number of plates (one variable), and the batch time (one decision variable). In comparison, new algorithm involves only two decision variables (N and R_0). (In the short-cut method, the number of plates N is not an integer variable but a real number representing theoretical number of plates.) Also, the new algorithm is found to be at least 6 times faster than the collocation discretization and NLP optimization approach. Dimensionality of the problem reduces considerably with the use of the new algorithm and results in great savings in computational time.

Conclusions

This article presented a novel approach for the solution of optimal design-control problems in batch distillation. The commonly employed techniques for solution of these problems have a number of shortcomings. This new approach is a combination of the maximum principle and NLP optimization, and was shown to circumvent the problems encountered by the two techniques and reduced the dimensionality of the prob-

Table 4. Input Data for the Test Problems

No.	Source	Objective	Rel. Vol.	Feed Comp.	Specifications	Cost Coeff.
a	Diwekar et al. (1987)	Maximum Distillate	2.0 1.5 1.0 0.5	0.25 0.25 0.25 0.25	$N=9+1$; $V=110$ $F=200$; $T=1$ $x_D^*=0.98$	
b	Coward (1967)	Minimum Time	2.0 1.0	0.4 0.6	$N=5$; $V=143.1$ $F=100$; $D_T=40$ $x_D^*=0.85$	
c	Logsdon et al. (1990)	Maximum Profit	1.5 1.0	0.5 0.5	$N=20$; $V=120$ $F=100$; $t_s=1$ $x_D^*=0.98$	$K_1=1{,}500$ $K_2=9{,}500$ $K_3=180$; $P_r/C_0=41/10$
d	Logsdon et al. (1990)	Maximum Profit (R_t bounded)	1.5 1.0	0.5 0.5	$N=20$; $V=120$ $F=100$; $t_s=1$ $x_D^*=0.98$	$K_1=1{,}500$ $K_2=9{,}500$ $K_3=180$; $P_r/C_0=41/10$

lem considerably. The new algorithm combined with the versatility of the short-cut method enabled a unified approach for solving optimization and optimal control problems for all the different operating conditions and different objective functions. The power of the new algorithm was demonstrated in the light of a number of examples reported in the literature. It was also shown that the solution for different classes of problems in optimal control of batch distillation columns has the maximum distillate problem embedded in it.

Notation

A_{ki} = coefficients arising from differentiating the Lagrange polynomial
B_t = amount remaining in the still at time t, mol
C_1 = constant in Hengestebeck-Geddes' equation
D_t = total distillate at time t, mol
F = total feed, mol
(L) = lower bound
m = total number of constraints $m=m_1+m_2$
m_1 = number of equality constraints
m_2 = number of inequality constraints
n = number of components
N = number of plates
$n\mathrm{col}$ = number of collocation points
$N_{\min}$ = minimum number of plates
$N_{\min f}$ = minimum number of plates at the terminal condition
nx = number of state variables $\bar{x}$
$R_{\max}$ = maximum initial reflux ratio for variable reflux mode
$R_{\min}$ = minimum reflux ratio
$R_{\min g}$ = minimum reflux ratio given by the Gilliland correlation
$R_{\min u}$ = minimum reflux ratio given by the Underwood equations
R_t = reflux ratio at time t
T = batch time, h
t_s = setup time, h
x_t^i = state variable i at time t from the vector $\bar{x}_t$
x_{initial}^i = initial value of state variable i from the vector $\bar{x}_{\mathrm{initial}}$
$x_B^{(i)}$ = still composition for component i
$x_{D\mathrm{ave}}$ = average distillate composition for the key component
x_D^* = specified average distillate composition for the key component
$x_D^{(i)}$ = distillate composition for component i
$x_F^{(i)}$ = feed composition for component i
(U) = upper bound
V = vapor boil-up rate, mol/h
w_i = weighing factor
z_t^i = adjoint variable i at time t from the vector $\bar{z}_t$

Greek letters

α_i = relative volatility of component i
$\bar{\lambda}$ = vector of Lagrange multipliers $[\bar{\lambda}_1, \bar{\lambda}_2]$
$\bar{\lambda}_1$ = vector of Lagrange multipliers for the equality constraints
$\bar{\lambda}_2$ = vector of Lagrange multipliers for the inequality constraints
$\bar{\mu}$ = scalar decision variable vector
ϕ_i = Underwood's constant
θ_t = control variable at time t

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