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

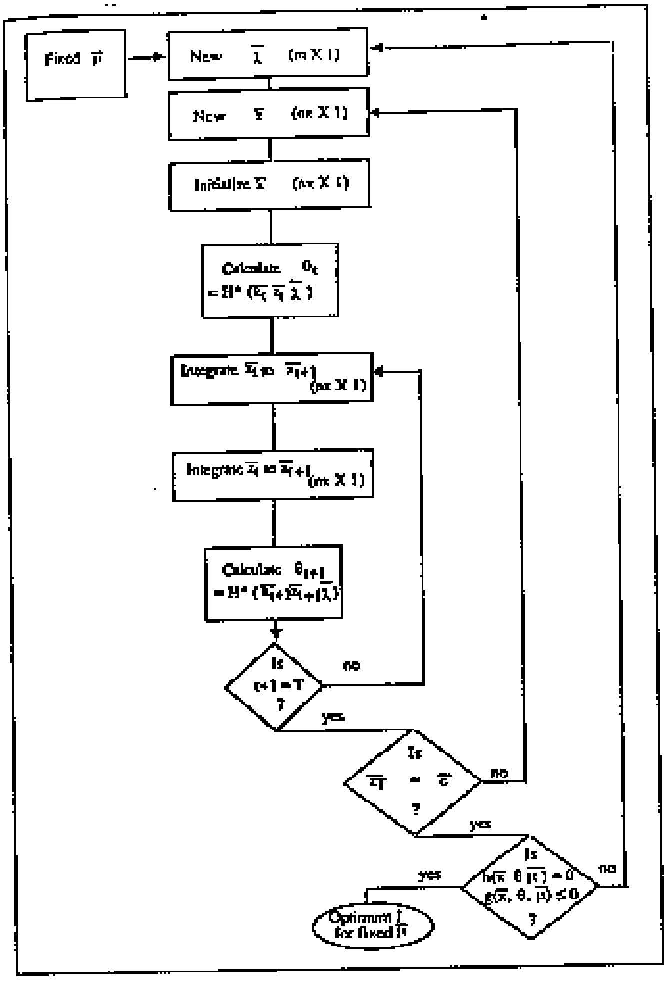

Figure 1. Solution using the maximum principle.

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

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

where J is the objective function given by Eq. 1, $\overline{x}_t$ is the state vector ($nx \times 1$ dimensional) at any time t, θ_t is the control vector, and $\overline{\mu}$ 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 $\overline{\mu}(L)$ represent the lower bounds on the control variables θ_t and the scalar variable μ, respectively, and $\theta(U)$, $\overline{\mu}(U)$ are the upper bounds for the same.

In the absence of the scalar variable vector $\overline{\mu}$, 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 ($\overline{\mu}$) only, not the complete DAOP described in the previous section. Figure 1 shows the solution to the DAOP for a fixed $\overline{\mu}$ based on the formulation given below.

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

subject to

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

$$h(\overline{x}_t, \theta_t, \overline{\mu}) = 0 \quad (7)$$

$$g(\overline{x}_t, \theta_t, \overline{\mu}) \le 0 \quad (8)$$

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

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

The righthand side of Eq. 5 represents the *linear objective function in terms of the final values* of $\overline{x}$ and values of $\overline{c}$, where $\overline{c}$ 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:

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

subject to

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

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

where

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

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

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

Differential Material Balance Equation

$$x_{B_{new}}^{(i)} = x_{B_{old}}^{(i)} + \frac{\Delta x_B^{(1)} (x_D^{(i)} - x_B^{(i)})_{old}}{(x_D^{(1)} - x_B^{(1)})_{old}}, \quad i = 1, 2, \ldots, n$$

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.

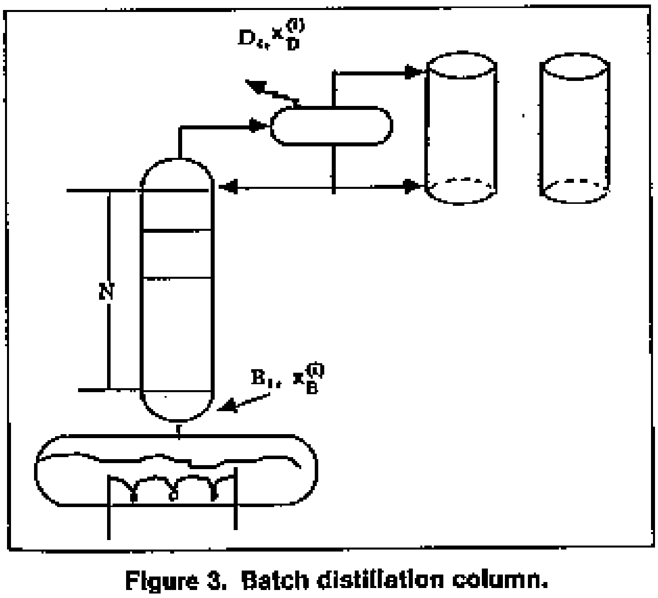

Figure 3. Batch distillation column.

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 ($\overline{z}_0 = \overline{c}$) 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 $\overline{\mu}$ 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:

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

subject to

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

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

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

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

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

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

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

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

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:

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

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:

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

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

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

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;

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

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.

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

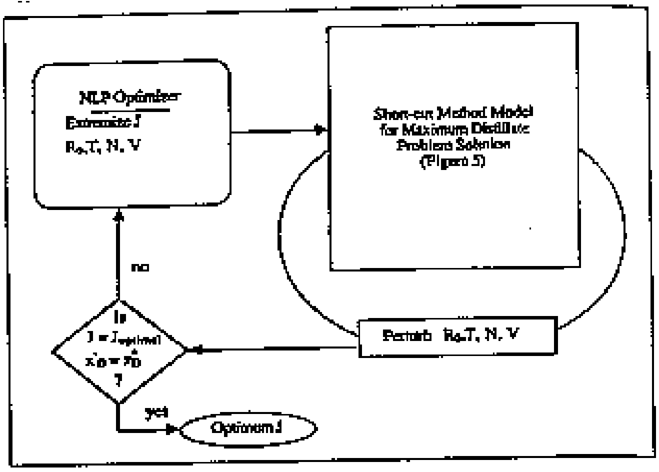

Figure 4. Combining maximum principle and NLP optimization techniques.

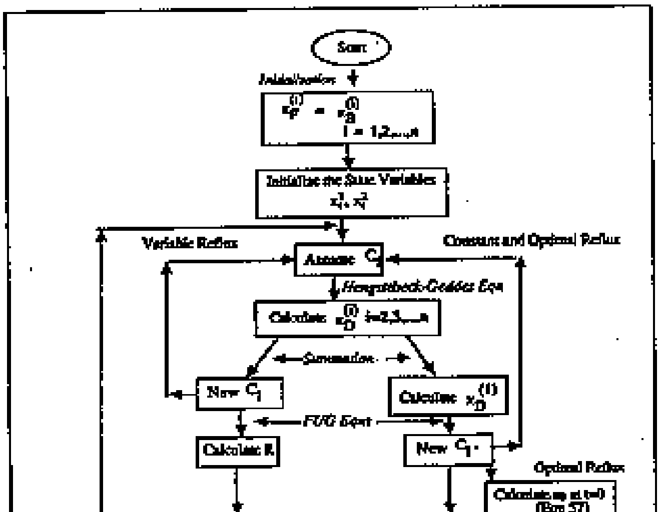

Figure 5. Unified short-cut model for NLP optimization.

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

	Variable Reflux	Constant Reflux	Optimal Reflux
		Differential Material Balance Equation	
		$x^{(i)}_{B_{new}} = x^{(i)}_{B_{old}} + \frac{\Delta x^{(1)}_B (x^{(i)}_B - x^{(i)}_D)_{old}}{(x^{(1)}_B - x^{(1)}_D)_{old}}$, $i = 1, 2, \ldots, n$	
		Hengestebeck-Geddes' Equation	
		$x^{(i)}_D = \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x^{(1)}_D}{x^{(1)}_B} x^{(i)}_B$, $i = 2, 3, \ldots, n$	
Unknowns	R, C_1	C_1, $x^{(1)}_D$	R, C_1, $x^{(1)}_D$
		Summation of Fractions	
		$\sum_{i=1}^{n} x^{(i)}_D = 1$	
	C_1 Estimation $\sum_{i=1}^{n} \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x^{(1)}_D}{x^{(1)}_B} x^{(i)}_B = 1$	$x^{(1)}_D$ Estimation $x^{(1)}_D = \frac{1}{\sum_{i=1}^{n} \left(\frac{\alpha_i}{\alpha_1}\right)^{C_1} \frac{x^{(i)}_B}{x^{(1)}_B}}$	
		Fenske Equation	
		$N_{min} = C_1$	
		Underwood Equations	
		$\sum_{i=1}^{n} \frac{\alpha_i x^{(i)}_B}{\alpha_i - \phi} = 0$; $R_{min_u} + 1 = \sum_{i=1}^{n} \frac{\alpha_i x^{(i)}_D}{\alpha_i - \phi}$	
		Gilliland Correlation	
	R Estimation $R = F(N, N_{min}, R_{min_u})$	C_1 Estimation $R_{min_g} = F(N, N_{min}, R)$ $\frac{R_{min_g}}{R} - \frac{R_{min_u}}{R} = 0$	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:

$$R_t = \frac{B_t - z_t(x^{(1)}_D - x^{(1)}_B)}{z_t \frac{\partial x^{(1)}_D}{\partial R_t}} - 1 \quad \text{for} \quad R_t \leq R(U)$$
$$R_t = R(U) \quad \text{for} \quad R_t > R(U) \tag{57}$$

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 op-

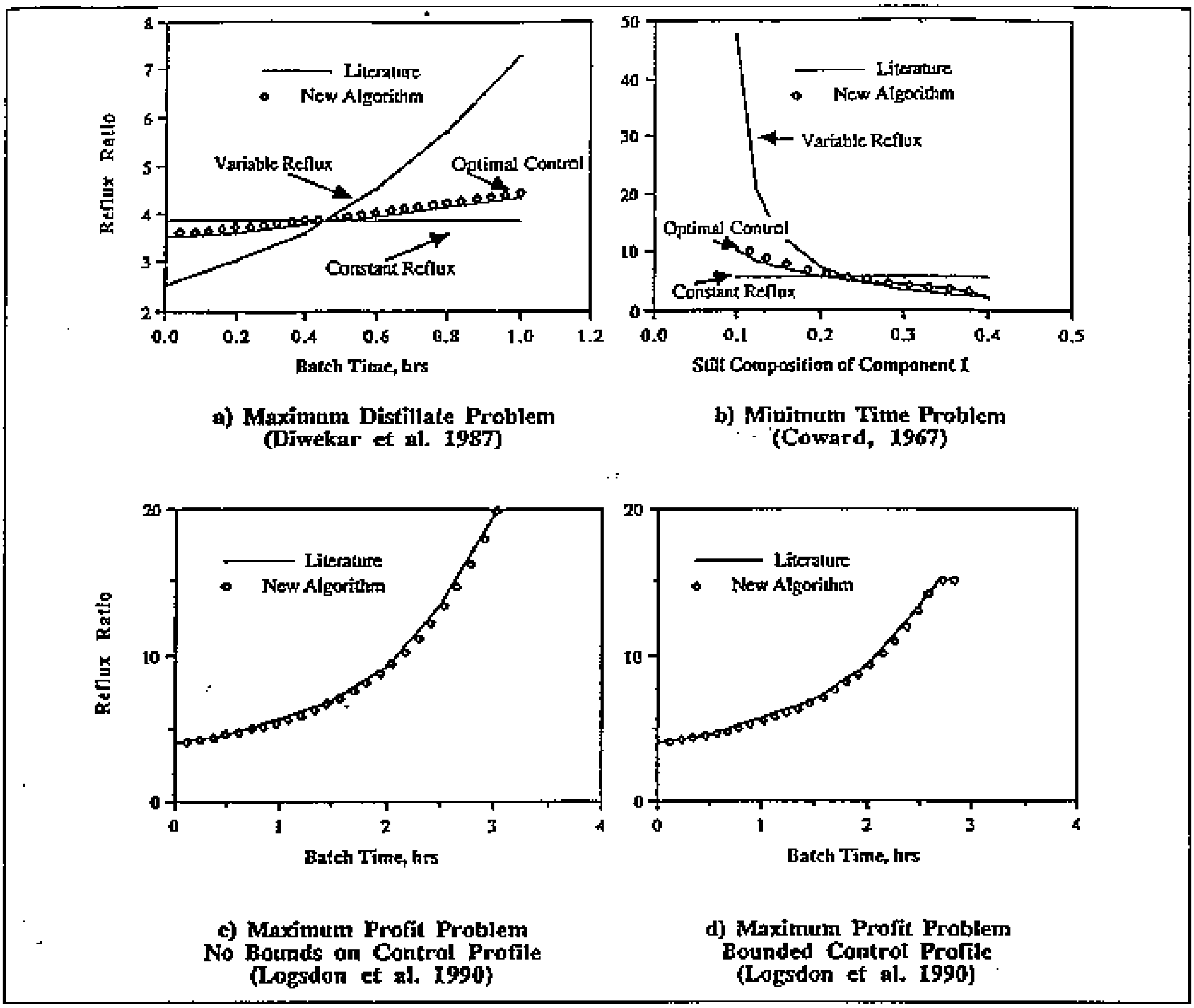

Figure 6. Solution for different DAOPs in batch distillation.

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-

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