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**NEW ERA IN BATCH DISTILLATION: COMPUTER
AIDED ANALYSIS, OPTIMAL DESIGN AND CONTROL**

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CONTENTS

- Abstract
- 1. Introduction
- 2. Theoretical Analysis
 - 2.1. Simple Distillation
 - 2.2. Operating Modes
 - 2.2.1 Constant Reflux Mode
 - 2.2.2 Variable Reflux Mode
 - 2.2.3 Optimal Reflux Mode
- 3. Hierarchy of Models
 - 3.1. Rigorous Model
 - 3.2. Low Holdup Semi-Rigorous Model
 - 3.3. Shortcut Model and Feasibility Considerations
 - 3.4. Collocation-based Models
- 4. Optimization and Optimal Control Problems
 - 4.1. Optimal Control Problems
 - 4.1.1 Performance Indices for Optimal Control Problems
 - 4.1.2 Solution Techniques

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- 4.2. Closed-Loop Control
5. Emerging Batch Columns, Complex Systems, and Synthesis
 - 5.1. Emerging Batch Columns
 - 5.1.1. Off-on Recycling Batch Distillation
 - 5.1.2. Batch Stripper
 - 5.1.3. Middle Vessel Column
 - 5.1.4. Multivessel Column
 - 5.2. Complex Batch Distillation Systems
 - 5.2.1. Azeotropic Batch Distillation
 - 5.2.2. Extractive Batch Distillation
 - 5.2.3. Reactive Batch Distillation
 - 5.3. Batch Distillation Synthesis
 - 5.4. Computer Aided Design Software
6. Conclusions
- Acknowledgements
- Notation
- References

ABSTRACT

The recent increase in the production of high value-added, low-volume specialty chemicals and biochemicals has generated a renewed interest in batch processing technologies. Batch distillation is an important unit operation in the batch processing industry and is most widely used. The flexibility of batch distillation, combined with the inherent unsteady nature of the process, poses challenging design and operation problems. This paper presents a complete review of batch distillation starting from the very first analysis in 1902 by Lord Rayleigh to the current state of the art. The paper will (a) introduce the various operating modes, (b) examine the challenges involved in rigorous modeling of batch distillation column dynamics, (c) provide a hierarchy of models of varying complexity and rigor, (d) present approaches to the optimal design and control of batch distillation columns and highlight the differences *vis-à-vis* continuous distillation columns, (e) analyze complex systems, (f) present methods to synthesize complex column designs, and (g) present an overview of available software packages for design, optimization, and control of batch distillation columns.

1. INTRODUCTION

"In the early days of chemical reaction engineering in the 1950s students might well have gained the impression that the ultimate mission of the chemical engineer was to transform old-fashioned batch processes into modern continuous ones.

With such a perspective it would be surprising to find that, today thirty years later, a significant portion of the world's chemical production by volume and a much larger proportion by value is still made in batch plants and it does not seem likely that this proportion will decline."

Rippon (1983)

Batch processing is the main feature of the pharmaceutical, biochemical, and specialty chemical industries. Batch units are also used in other chemical industries where small quantities of materials are to be handled in irregularly scheduled periods, and are preferable to continuous units when the feed composition varies widely from period to period, or where completely different feed stocks need to be handled.

Batch distillation is the oldest separation process and the most widely used unit operation in the batch industry. Theoretical studies on batch distillation began as a simple distillation still in a laboratory; Figure 1 shows

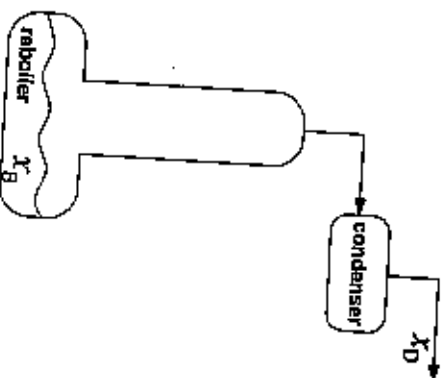


Fig. 1: A schematic diagram of a simple distillation operation.

a schematic illustration of such a still initially filled with a feed mixture which evaporates and leaves the still in the vapor form. This vapor, which is richer in the more volatile component, is collected in the condenser at the top and accumulated in a receiver (not shown in this figure). In this operation no liquid is refluxed back to the still, and no plates or packing materials are present inside the still. This simple distillation still is an example of a batch operation, often referred to as *Rapley's distillator* because of his pioneering theoretical work in simple distillation (Rapley, 1902). The concept of reflux and the use of accessories such as plates and packing materials to increase the mass transfer converts this simple still into a distillation column. Figure 2 represents a conventional batch distillation column with reflux and multiple stages. This batch column consists of a reboiler at the bottom, a condenser and a condenser at the top. The column generally consists of a cylindrical structure divided into sections by a series of perforated plates, trays, or packing materials that permit the upward flow of vapor. As the liquid reflux flows down the column, the vapor and liquid come into contact on each stage where the mass transfer takes place. Consequently, the rising vapor becomes

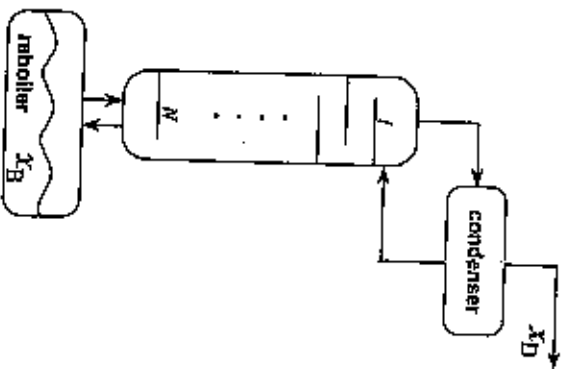


Fig. 2: A schematic diagram of a conventional batch distillation operation.

richer in the more volatile component, while the descending liquid becomes correspondingly weaker. Because this column essentially performs the rectifying operation, it is often called a batch rectifier.

Batch distillation is preferable to continuous distillation when small quantities of high value-added chemicals need to be separated. The most outstanding feature of batch distillation is its flexibility. This flexibility allows one to deal with uncertainties in feed stocks or product specifications. In addition, one can handle several mixtures just by switching the column's operating conditions. The basic difference between batch rectification and continuous distillation is that in continuous distillation the feed is continuously entering the column, while in batch distillation the feed is charged into the reboiler at the beginning of the operation. Also, while the top products are removed continuously in both the batch and the continuous operations, there is no continuous bottom product withdrawal in a conventional batch operation. Since the total product flow rate in a continuous operation equals that of incoming feed or feeds, the process reaches steady state and lacks the degree of freedom in the relationship between the feeds and the products. In batch distillation, on the other hand, the reboiler gets depleted over time, so the process is of unsteady-state nature. The batch column can be operated under the following different operating conditions or policies:

- Constant reflux and variable product composition,
- Variable reflux and constant product composition of the key component, and
- Optimal reflux and optimal product composition.

In the constant reflux policy, the instantaneous composition of the distillate keeps changing since the bottom still composition of the more volatile component is continuously depleted. On the other hand, in the variable reflux policy, the composition of the key component in the distillate can be kept constant by increasing the reflux ratio. There is a third policy of operation known as the optimal reflux policy that is neither the constant reflux policy nor the variable reflux policy. Instead, this operating policy exploits the difference between the two operating modes. Thus, the optimal is based on the ability of the process to yield the most profitable operation.

The transient nature of batch distillation allows configuring the column in a number of different ways, some of which are shown in Figure 3 (Diwekar,

1996). The column in Figure 3a, as explained, is the conventional batch distillation column with the reboiler at the bottom and the condenser at the top, which essentially performs the rectifying operation. A single column can be used to separate several products using the multi-fraction operation of

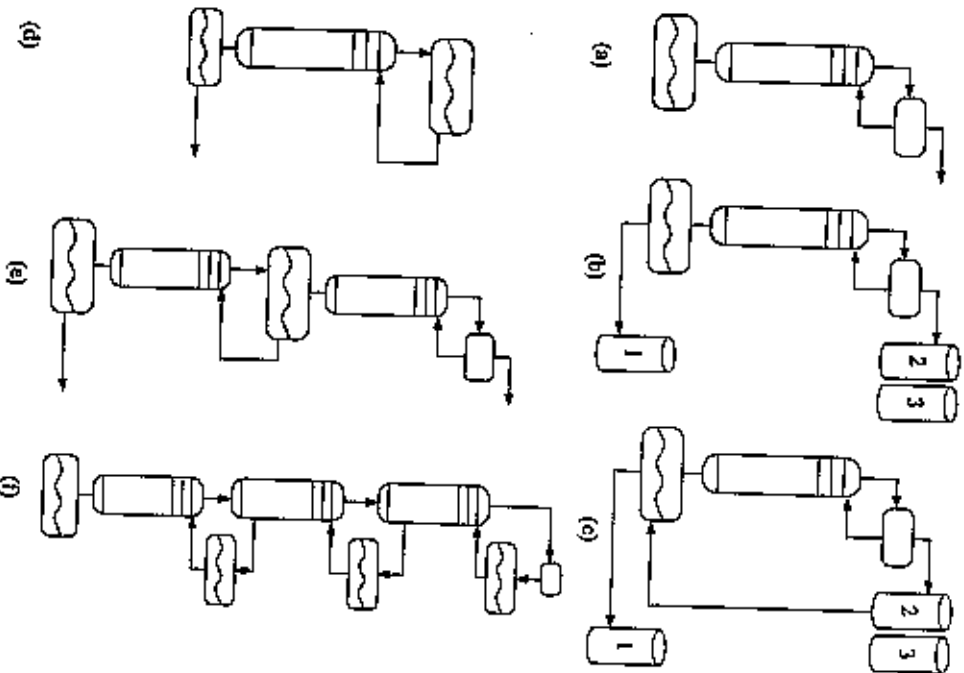


Fig. 3: Examples of ways to configure the batch distillation column.

batch distillation presented in Figure 3b. Some cuts may be desired and others may be intermediate products. These intermediate fractions can be recycled to maximize profits and/or minimize wastes. Figure 3c shows a periodic operation in which each charge consists of a fresh feed stock mixed with the recycled off-specification material from the previous charge. Configurations in Figure 3b and 3c can be implemented in an optimal campaign structure (Walge and Rokkati, 1998). Figure 3d represents a stripping column for separating the heavy product as the bottom product where the liquid feed is initially charged into the top. In 1994 Davidson *et al.* presented a batch distillation column that has both stripping and rectifying sections embedded in it (Figure 3e). Although this column has not been investigated completely, recent studies demonstrated that it provides added flexibility for the batch distillation operation. Recently Skogestad *et al.* (1997) described a new column configuration called a multi-vessel column (Figure 3f), which is similar to the MEBDS (multi-effect batch distillation system) of Hasace *et al.* (1995), and showed that the column can obtain purer products at the end of a total reflux operation. These emerging designs play an important role in separation of complex systems like azeotropic, extractive, and reactive batch distillation systems. The batch rectifier configuration for such separations may be very restrictive and expensive.

These emerging designs, combined with different possible operating modes similar to the ones described earlier for the rectifier, provide greater flexibility, but result in a large number of column configurations. Because of the unsteady-state nature of the operation, embedded in the design problem is the optimal control problem of deciding time-dependent variables such as reflux ratios, reboil ratios, vapor flow rates, and/or vessel holdups. Given this flexibility, batch distillation poses a difficult synthesis problem involving the selection of optimal column configurations and the optimal operating condition. Complex systems such as azeotropic, extractive, and reactive distillation add another dimension to the synthesis problems as the cuts (fractions) in the multi-fraction operation can have significantly different characteristics depending on the feed mixture of these systems.

The complexity in design, synthesis, and analysis of batch distillation due to (1) unsteady-state nature, (2) operational flexibility, and (3) emerging design, can only be handled systematically using the computer-aided design techniques and recently developed software tools.

This paper presents a complete review of batch distillation starting from the first analysis in 1902 by Lord Rayleigh to the current state-of-the-art

computer-aided design techniques. The paper introduces an early theoretical analysis of simple distillation and various operating policies in Section 2. Section 3 examines the challenges involved in rigorous modelling of batch distillation dynamics and provides a hierarchy of models of varying complexity and rigor. Recent advances in optimal design and control problems are discussed in Section 4. Emerging columns, complex systems, and batch synthesis are described in Section 5, followed by an overview of available software packages. The last section provides the overall conclusions and future research directions.

2. THEORETICAL ANALYSIS

This section presents early theoretical analysis of simple distillation, which was first analysed by Rayleigh (1902). The limitations of simple distillation that led to the development of the batch rectifier are discussed. The operational flexibility of batch distillation in terms of operational policies is also presented.

2.1 Simple Distillation

The analysis of simple distillation presented by Lord Rayleigh in 1902 marks the earliest theoretical work on batch distillation. Simple distillation, also called Rayleigh distillation or differential distillation, is the most elementary example of batch distillation. As shown in Figure 1, the vapor is removed from the still during each time interval and is condensed in the condenser. The more volatile component in the vapor is richer than the liquid remaining in the still. Over time, the liquid remaining in the still begins to experience a decline in the concentration of the more volatile component, while the distillate collected in the condenser becomes progressively enriched in the more volatile component. No reflux is returned to the still, and no stages or packing materials are provided inside the column. Therefore, various operating policies are not applicable to this distillation system.

The early analysis of this process for a binary system, proposed by Rayleigh, is given below. Let F be the initial binary feed to the still (moles), and x_F be the mole fraction of the more volatile component A in the feed. Let B be the amount of components remaining in the still, x_B the mole fraction of component A in the still, and x_D the mole fraction of component A in the

vapor phase. The differential material balance for component A can then be written as:

$$x_D dB = d(Bx_D) = B dx_D + x_D dB \quad (1)$$

giving:

$$\int_F^B \frac{dB}{B} = \int_{x_D}^{x_D} \frac{dx_D}{x_D - x_B} \quad (2)$$

or

$$\ln\left(\frac{B}{F}\right) = \int_{x_D}^{x_D} \frac{dx_D}{x_D - x_B} \quad (3)$$

In this simple distillation process, it is assumed that the vapor formed within a short period is in thermodynamic equilibrium with the liquid. Hence, the vapor composition x_D is related to the liquid composition x_B by an equilibrium relation of the form $x_D = f(x_B)$. The exact relationship for a particular mixture may be obtained from a thermodynamic analysis depending on temperature and pressure. For a system following the ideal behavior given by Raoult's law, the equilibrium relationship between the vapor composition y (or x_D) and liquid composition x (or x_B) of the more volatile component in a binary mixture can be approximated using the concept of constant relative volatility (α), and is given by:

$$y = \frac{\alpha x}{(\alpha - 1)x + 1} \quad (4)$$

Substitution of the above equation in Equation 3 results in:

$$\ln\left(\frac{B}{F}\right) = \frac{1}{\alpha - 1} \ln \left[\frac{x_B (1 - x_F)}{x_F (1 - x_B)} \right] + \ln \left[\frac{1 - x_F}{1 - x_B} \right] \quad (5)$$

Although the analysis of simple distillation historically represents the theoretical start of batch distillation research, a complete separation using this process is impossible unless the relative volatility of the mixture is infinite.

Therefore, the application of simple distillation is restricted to laboratory scale distillation, where high purities are not required, or when the mixture is easily separable.

To obtain products with high purity, multistage batch distillation with reflux has been used. As shown in Figure 2, the batch rectifier comprises multiple thermodynamic stages (manifested by internal trays or packings) inside the rectifying section. The feed is normally charged to the reboiler at the beginning of the operation. Whereas the top products are removed continuously, there is no bottom product withdrawal in batch distillation, and the reboiler gets depleted over time. This makes batch distillation an unsteady-state operation.

2.2 Operating Modes

Although simple distillation marks the first analysis of batch distillation process, the graphical analysis presented by McCabe and Thiele (1925) provided the basis for analyzing batch distillation operating modes. The difference between simple distillation and batch distillation operations is due to the presence of reflux and column internals. They suggested a graphical method (Figure 4) to calculate this relation using the following procedure.

In the McCabe and Thiele method, the overall material balance with no holdup is considered from the condenser to the j -th plate. This leads to the following operating equation:

$$y_j = \frac{R}{R+1}x_{j-1} + \frac{1}{R+1}x_D \quad (6)$$

This operating equation represents a line through the point y_j ($x_{j-1} = x_D$) with a slope of $\frac{R}{R+1}$. Starting from this point (x_D, x_D), which corresponds to the distillate composition, Equation 6 and the equilibrium curve between y and x can be recursively used from the top plate 1 to the reboiler (the reboiler can be considered as the $(N+1)$ -th plate). This procedure relates the distillate composition x_D to the still composition x_B through the number of stages.

In the case of batch distillation, however, the still composition x_B does not remain constant as observed in continuous distillation, and thus the instantaneous distillate composition y_B is also changing. This necessitates the

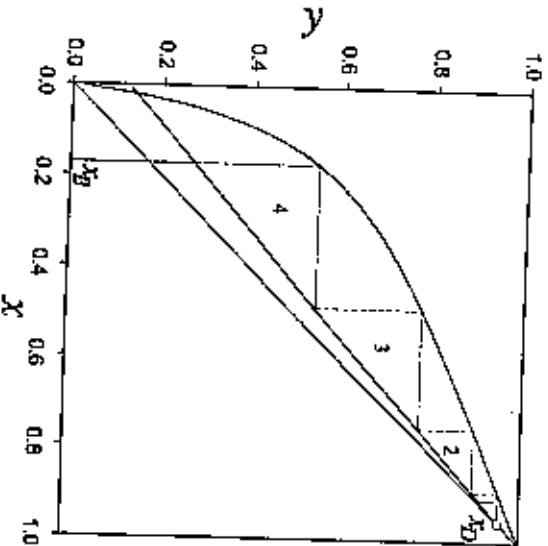


Fig. 4: McCabe-Thiele method for plate-to-plate calculations.

use of the recursive scheme several times. If the scheme is used, while keeping the reflux ratio constant throughout the operation just like normal continuous distillation, the composition of the distillate keeps changing (Figure 5). This is the constant reflux mode of operation. On the other hand, the composition of the key component in the distillate can be maintained as constant by changing the reflux resulting in the variable reflux mode of operation. In addition, there is a third mode of operation of batch distillation that is neither the constant reflux, nor the variable reflux policy. This type of operation is known as the optimal reflux or optimal control policy, designed to optimize a particular peak mode like the maximum distillate, minimum time, or maximum profit functions.

Stillier operating modes are also observed in emerging batch distillation columns. For example a stripper can also have three operating modes: (a) constant reboil ratio, (b) variable reboil ratio, and (c) optimal reboil ratio modes (Loker and Diwekar, 1997; Sorensen, 1999). For a middle vessel column, the combination of the three reflux and three reboil policies results

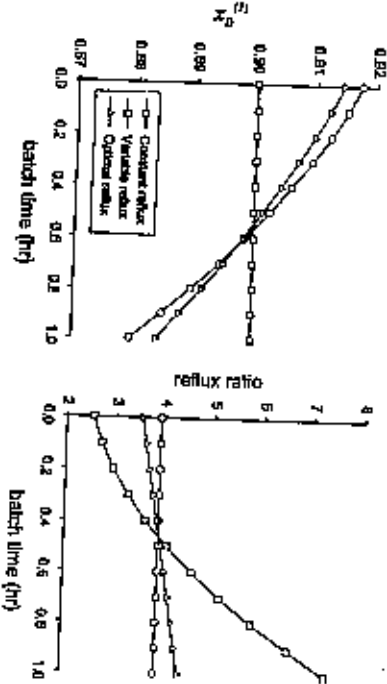


Fig. 5: Three operating modes for a batch rectifier.

in at least nine possible operating policies. The operating modes of a multivessel column can be derived based on the middle vessel column, but this column configuration requires additional considerations with respect to operating variables such as the holdup in each vessel. The total reflux mode can be also considered especially in the middle vessel and multivessel columns. As these column designs are still under extensive research, the early analysis of operating modes is mainly restricted to the batch rectifier and is discussed below.

2.2.1 Constant Reflux Mode

Smoker and Rose (1940) presented the first analysis of the constant reflux operation of a binary batch distillation with no holdup. They used the Rayleigh equation in conjunction with the McCabe-Thiele graphical method (McCabe and Thiele, 1925) to capture the dynamics of the batch distillation column. In their procedure, the relationship between x_D and x_B is recursively determined by the McCabe-Thiele graphical method. Then, the right hand side of the Rayleigh equation (Equation 3) is integrated graphically by plotting $\frac{1}{x_D - x_B}$ versus x_B . The area under the curve between the feed composition x_F and the still composition x_B now gives the value of the integral, which is in Eq. (7). The average composition of the distillate can be obtained from the following equation:

$$x_{D,avg} = \frac{F x_F - B x_B}{F - B} \tag{7}$$

Although Smoker and Rose presented the calculation method independent of time, the time can be introduced through the vapor boilup rate V of the reboiler. The resulting equation for determining batch time is given by:

$$T = \frac{R+1}{V} (F - B) = \frac{R+1}{V} D \tag{8}$$

This operation policy is the easiest one and is commonly used. In many binary and ternary distillation cases, little improvements can be obtained from this operation mode to the variable reflux mode or the optimal reflux mode (Coward, 1966; Lyben, 1988; Al-Tuwaim and Layben, 1991; Espinose and Salomone, 1999), which is described below.

2.2.2 Variable Reflux Mode

In 1937, Bogart presented the first analysis of the variable reflux policy for a binary system. The steps involved in the calculation procedure for the variable reflux mode are similar to those in the case of the constant reflux mode; however, in the variable reflux case, the reflux ratio is varied instead of the distillate composition at each step. Moreover, the Rayleigh equation, though valid for the variable reflux condition, takes a simplified form. Since the distillate composition remains constant (remember that we are considering binary systems here) throughout the operation, the Rayleigh equation reduces to the following equation.

$$\frac{B}{F} = \frac{x_D - x_F}{x_D - x_B} \tag{9}$$

The second step is to establish the relation between R and x_B using the McCabe-Thiele graphical method. Several values of R are selected, operating lines are drawn through the fixed point (x_B, x_D) with the slope of $\frac{R}{R+1}$, and steps are drawn between the operating line and the equilibrium curve to get the bottom composition (x_B) . This recursive scheme is repeated until the desired stopping criteria is met, and thus B and x_B can be found at each value of the reflux ratio. The time required for this operation at a given product purity is calculated by plotting the quantity $\frac{Bx_D - Fx_F}{(x_B - x_F)^2}$ versus x_B in the

following equation and then finding the area under the curve.

$$T = \int_{x_F}^{x_D} \frac{R+1}{V} \frac{F(x_D - x_F)}{(x_D - x_B)^2} dx_B \quad (10)$$

The variable reflux operation policy is commonly used with a feedback control strategy because the reflux ratio is constantly adjusted to keep the distillate composition constant (Quintero-Marmol *et al.*, 1991; Quintero-Marmol and Luyben, 1992; Baroña and Berio, 1998). Section 4.2 presents detailed description of the control strategy involved in this operating mode.

2.2.3 Optimal Reflux Mode

The optimal reflux policy is essentially a *trade-off* between the two operating modes, and is based on ability to yield the most profitable operation from optimal performance. The calculation of this policy is a difficult problem and relies on optimal control theory. The batch distillation literature is rich in papers on this policy. Therefore, a separate section (Section 4.1) is dedicated to discussing the solution procedures for this operating mode. There are different kinds of optimal reflux policies depending on the indices of performance chosen as the objectives. The indices used in practice generally include the minimum time, maximum distillate, or maximum profit functions.

Although the first optimal reflux policy was discussed as early as 1963 (Converse and Gross, 1963), the real implementation of this procedure has only been possible recently because of the advent of computers.

3 HIERARCHY OF MODELS

As seen in Section 2, the earlier models of the batch rectifier were built on assumptions of negligible liquid holdup and ideal binary systems. Computers have played an important role in relaxing these assumptions, especially the negligible holdup assumption. The first rigorous model of batch distillation with constant holdup was published by Muecke and Dery (1960), which was developed using analogue computers. Distefano analyzed the numerical differential equations for multicomponent batch distillation in 1968 for the first time. The rigorous models of batch distillation in current state of the art

computer packages are based on Distefano's pioneering work. However, it was also acknowledged that due to the severe transients in batch distillation, a hierarchy of models is necessary to capture the dynamics of this flexible operation (Diwekar, 1996). This section presents the hierarchy of models ranging from the rigorous model similar to the one presented by Distefano to the simplest shortcut model.

3.1 Rigorous Model

A rigorous model in batch distillation involves consideration of column dynamics along with the reboiler and condenser dynamics. Detailed analysis of the characteristics of differential mass and energy balances associated with the complete dynamics of a multicomponent batch distillation column was presented by Distefano (1968). Distefano pointed out that the system of equations presented for batch distillation is much more difficult to solve than that of the dynamics of continuous distillation and that this is due to several factors. For example, in the case of batch distillation plate holdup, it is generally much smaller than the reboiler holdup, while in continuous distillation, the ratio of the reboiler holdup to the plate holdup is not nearly as great. In addition, in batch distillation severe transients can occur, unlike continuous distillation where the variations are relatively small. Distefano's work forms the basis for almost all of the later work on rigorous modeling of batch distillation columns (Boston *et al.*, 1983; Diwekar, 1998; Diwekar and Madhavan, 1991), and this model is presented below.

Figure 6 represents a schematic of a batch distillation column, where the holdup on each plate is responsible for the dynamics of each plate. For an arbitrary plate j , the total mass, component, and energy balances yield the governing equations, summarized in Table 1. This table lists all the equations involved in the dynamic analysis of the batch column and the assumptions behind these equations.

As the governing equations represent a generalized form of the batch rectifying column, the treatment of the individual operating mode, such as the constant reflux, variable reflux, or optimal reflux modes, exploits the same governing equations, but with different specifications. Furthermore, the governing equations of the stripper, middle vessel column, and multivessel column can be similarly derived.

In recent years, researchers have relaxed some of the assumptions specified in Table 1 in order to include rigorous aspects of tray dynamics

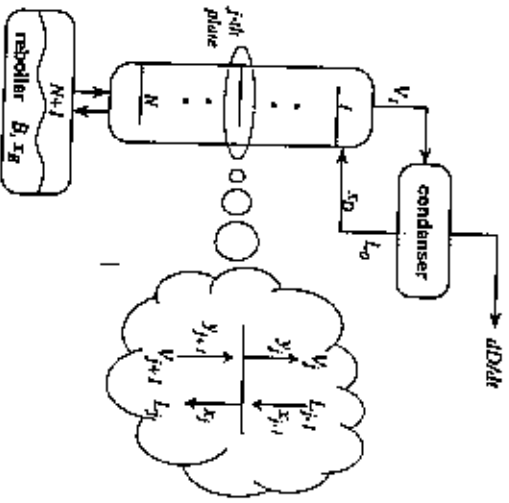


Fig. 6: Schematic of a batch distillation column.

(Tomazi, 1997) and holdup effects (Mujtaba and Marchetti, 1998). Tomazi showed that the limitations of tray hydraulics decrease the yield and capacity mainly due to the failure of the intermediate product cut to meet its purity specification. One of the long debated issues in batch distillation is the holdup effect. It is reported that increasing holdup can improve column performance in some cases but degrade it in others. Mujtaba and Marchetti (1998) revisited this problem for a binary system and provided a unified result of the holdup effect in terms of the degree of difficulty of separation (q) and the minimum time. It is found that for easy separations (typically $q < 0.6$), increasing holdup improves column performance in the context of minimum batch time but deteriorates the performance for difficult separations.

From the system of differential equations in Table 1, one can easily see that there is no analytical solution to the problem, and one must resort to numerical solution techniques. The governing differential equations of batch distillation often fall into the category of stiff differential equations. The solution of stiff differential equations contains a component that contributes very little to the solution but can cause errors by accumulating over time.

Table 1
The complete column dynamics for a rigorous model.

Assumptions
<ul style="list-style-type: none"> • Negligible vapor holdup • Adiabatic operation • Theoretical plates • Constant molar holdup • Finite difference approximations for the enthalpy changes
Condenser and Accumulator Dynamics
$\frac{dx_D}{dt} = \frac{V_1}{R D} (y_1^D - x_D^D), \quad t = 1, 2, \dots, n$
Plate Dynamics
$\frac{dy_j^D}{dt} = \frac{1}{V_j} [V_{j+1} y_{j+1}^D + L_j x_{j-1}^D - V_j y_j^D - L_j x_j^D], \quad t = 1, 2, \dots, n; j = 1, 2, \dots, N$
Reboiler Dynamics
$\frac{dx_B^D}{dt} = \frac{1}{V_B} [L_N (x_N^D - x_B^D) - V_B (y_B^D - x_B^D)], \quad t = 1, 2, \dots, n$
Flow Rate Calculations
<p>At the Top of the Column</p> $L_0 = R \frac{dx_D}{dt}, \quad V_1 = (R + 1) \frac{dx_D}{dt}$ <p>On the Plates</p> $L_j = V_{j+1} + L_{j-1} - V_j, \quad j = 1, 2, \dots, N$ $V_{j+1} = \frac{V_j}{\alpha_j} [W_j (L_j - L_j^0) + F_{j+1} (L_j - L_j^0) + H_j \delta_j], \quad j = 1, 2, \dots, N$ <p>At the Bottom of the Column</p> $\frac{dx_B^D}{dt} = L_N - V_B$
Heat Duty Calculations
<p>Condenser Duty</p> $Q_C = V_1 (T_1 - T_D) - H_D \delta_1 t_0$ <p>Reboiler Duty</p> $Q_R = V_B (T_B - T_R) - L_N \delta_1 t_0 + B \delta_1 t_0$ <p>Thermodynamic Models</p> <p>Equilibrium Relations</p> $y_j^D = f \left(\left(\frac{p_j^D}{p} \right)^k, T_{E,j}, P_j \right)$ <p>Enthalpy Calculations</p> $T_j = f \left(\left(\frac{p_j^D}{p} \right)^k, T_{E,j}, P_j \right)$ $H_j = f \left(\left(\frac{p_j^D}{p} \right)^k, T_{E,j}, P_j \right)$

resulting in a totally different solution. Most recent batch distillation codes (Boston *et al.*, 1983; Diwekar and Madhavan, 1991) use numerical methods based on BDF (backward difference formula), and one of the well known BDF techniques is the LSODE (Hindmarsh, 1980) method. Since the computational intensity of the stiff algorithms is generally more severe than the non-stiff algorithms, it is better to switch to non-stiff algorithms. The quantifying measures, such as the stiffness ratio SR (Frilayson, 1980) or computational stiffness $SC(t)$ (Cameron *et al.*, 1986) both based on eigenvalue

calculations, can be used to decide about this switching. However, eigenvalue calculations are computationally expensive and hence are not normally used for the large system of differential equations.

Stiff systems can also be defined as near-index systems (which is beyond the scope of this article), and high-index problems are infinitely stiff problems (Chung, 1991). It should be noted that for high-index systems, it is difficult to apply any numerical integration method unless the system is transformed in some ways to reduce the index of the system. This can happen in batch distillation of wide boiling systems or for columns where the holdup inside the column is significantly smaller than that of the still. The semi-rigorous model can be used to circumvent this problem.

3.2 Low Holdup Semi-Rigorous Model

For columns where the plate dynamics are significantly faster than the reboiler dynamics (due to very small plate holdups and/or wide boiling components), the stiff integrator often fails to find a solution (Diwekar, 1996, page 59). The solution to this problem is to split the system into two levels: (1) the reboiler, where the dynamics are slower, can be represented by differential equations, and (2) the rest of the column can be assumed to be in the quasi-steady state. Thus, the composition changes in the condenser and accumulator ($\frac{dx_D^{(i)}}{dt}$), the composition changes on plates ($\frac{dx_j^{(i)}}{dt}$), and the enthalpy changes in the condenser and on plates ($\delta_j T_D$ and $\delta_j T_j$) in Table 1 can be assumed zero. This results in a zero holdup model, so this approach can be used for simulating the semi-rigorous model of batch distillation.

Domenech and Engilbert (1981) developed a general simulation program of batch rectification, in which they considered a semi-rigorous model with the constant or variable reflux policy. Bernot *et al.* (1990, 1991) developed and compared semi-rigorous models of the batch reboiler and stripper for the behavior of multicomponent azeotropic distillation. Diwekar (1988, 1996) and Divakar and Madhavan (1991) developed the software packages, BATCH-DIST and MultiBatchDS, in which a semi-rigorous model is implemented.

The holdup effects can be neglected in a number of cases where this model approximates the column behavior accurately. This model provides a close approximation to the Rayleigh equation, and for complex systems (e.g. azeotropic systems) the synthesis procedures can be easily derived based on

the simple distillation residue curve maps (please refer Section 5.2 for details). However, note that this model involves an iterative solution of nonlinear plate-to-plate algebraic equations, which can be computationally less efficient than the rigorous model.

3.3 Shortcut Model and Feasibility Considerations

As seen in Section 3.1, the rigorous model of batch distillation operation involves a solution of several stiff differential equations. The computational intensity and memory requirement of the problem increase with an increase in the number of plates and components. The computational complexity associated with the rigorous model does not allow us to derive global properties such as feasible regions of operation, which are critical for optimization, optimal control, and synthesis problems. Even if such information is available, the computational costs of optimization, optimal control, or synthesis using the rigorous model are prohibitive. One way to deal with these problems associated with the rigorous model is to develop simplified models such as the shortcut model and the collocation-based model. These simplified models are abstractions of the rigorous model, and their accuracy depends on the simplifying assumptions embedded within them. The process of abstraction can be viewed as a trade-off between simplicity and accuracy. The usefulness of the abstracted model depends on the ease with which they can be analyzed for global behaviors without compromising accuracy. Moreover, the abstracted models are expected to be computationally simpler to analyze.

Development of shortcut models for batch distillation and their use in optimization and optimal control seems to be the recent trend in batch distillation (Chioiti and Imbarra, 1991; Al-Tuwain and Luyben, 1991; Zamur *et al.*, 1998). These models are either confined to binary (Chioiti and Imbarra, 1991) or ternary systems (Al-Tuwain and Luyben, 1991), or are applied to multiple task batch distillations (Zamur *et al.*, 1998) for the simulation.

The shortcut model of batch distillation proposed by Diwekar and coworkers (Diwekar, 1988; Diwekar and Madhavan, 1991) is based on the assumption that the batch distillation column can be considered equivalent to a continuous distillation column with changing feed at any instant. Since continuous distillation theory is well-developed and tested, the shortcut method of continuous distillation is modified for batch distillation, and the

compositions are updated using a finite difference approximation for the material balance (based on the Rayleigh equation). The other assumptions of the shortcut method include constant molar overflow and negligible plate holdups. The details of this method are described in the book by Diwekar (1996). As described earlier, the functional relationship between the distillate composition x_D and the bottom composition x_B is crucial for the simulation, and the FUG (Fenske-Underwood-Gilliland) method is used for estimating this relation.

Shortcut methods have also been modified to incorporate holdup issues using a compartmental modeling approach, and extended to complex mixtures containing binary and ternary azeotropes (Diwekar, 1991a; Kalagnanam and Diwekar, 1993). Recently, Lokar and Diwekar (1997) applied a similar shortcut approach to emerging batch columns such as the stripper and the middle vessel column.

The shortcut model is very useful in feasibility analysis. In order to maintain the feasibility of design, there are certain constraints on the variables, especially for the design variables such as the number of plates N and reflux ratio R . The shortcut model helps to identify these bounds on the design parameters. The bounds on the parameters depend on the operating modes. The feasible region of operation has been identified using the shortcut model by Diwekar and coworkers and is summarized in Table 2.

In this table, R_{min} is the Underwood minimum reflux ratio, which is different from R_{min} . R_{min} is defined as the value of R required to obtain the distillate composition of the key component equal to the specified average distillate composition (x_D^a) at the initial conditions for the given N . Recently,

Table 2

Feasible region for multicomponent batch distillation columns.

Variable Reflux	Constant Reflux	Optimal Reflux
Final Still Composition		
$0 \leq x_{A1}^{(1)} \leq x_D^{(1)}$		
Distillate Composition		
$x_D^{(1)} \leq x_D^a \leq 1$		
Reflux Ratio		
$R_{min} \leq R_{min} \leq R_{max}$	Range	$R_{min} \leq R \leq \inf$
Number of Plates		
$N_{min,1} \leq N$		$N_{min} \leq N$

Kim and Diwekar (2000) have defined new performance indices such as the N -feasibility index and the R -feasibility index for analyzing feasible regions of various column configurations. These new indices can identify distinctive feasibility regions for various configurations and provide useful guidelines for optimal column selection.

The shortcut model has been found to be extremely efficient and reasonably accurate for nearly-ideal mixtures and for columns with negligible holdup effects.

3.4 Collocation-based Models

The next simplified model in the simulation hierarchy is the reduced order model based on the orthogonal collocation approach. The collocation approach was first proposed in the context of continuous staged separation processes by Cho and Joseph (1983a,b). The collocation approach to model reduction is based on approximating the column stage variables by using polynomials rather than discrete functions of stages, and thus is widely used for packed batch column design. The orthogonal collocation technique can change partial differential equations to ordinary differential or algebraic equations, and ordinary differential equations (ODEs) to a set of algebraic equations. In the case of batch distillation, we encounter ordinary differential equations, and the orthogonal collocation technique can be used to reduce this system of ODEs into nonlinear algebraic equations.

Srivastava and Joseph (1984) developed the orthogonal collocation method of a simplified packed batch column using the 4th-order polynomial. Christensen and Jørgensen (1987) presented a collocation-based model of binary batch distillation having quasi steady-state trays or packings. This approach was extended to obtain the reduced order model of batch distillation by Diwekar (1988). For a quasi-steady state batch distillation with total reflux, Aly *et al.* (1990) used the Galerkin method as the weighting function over the finite elements. Even though the Galerkin method is one of the best known approximation methods for weighted residuals, this method is difficult to implement.

Note that the orthogonal collocation model can also be used to reduce the order of optimization problems. It is not always advantageous to convert ordinary differential equations to nonlinear algebraic equations. The converted large systems of algebraic equations are computationally time consuming. Instead of using the orthogonal collocation to reduce the ODEs to

nonlinear algebraic equations, one can use it to reduce the order of ODEs. For example, Diwekar (1988) developed a reduced order model of batch rectification, and Waige *et al.* (1997) combined the orthogonal collocation method and the finite element method for a packed reactive batch distillation to reduce the order of ODEs.

This model is especially useful when other simplified models cannot be used to describe the column (e.g. for highly nonideal systems or systems for which constant molar flow assumptions cannot be used).

4 OPTIMIZATION AND OPTIMAL CONTROL PROBLEMS

The previous sections concentrated on the design and simulation of batch distillation columns using a hierarchy of models. Optimal design and operation in a batch distillation process is challenging decision-making problems that involve several time-dependent and independent decisions in the face of operating and thermodynamic constraints. Mathematical optimization theory makes the decision-making process easier and systematic. With the advent of computers, it is possible to exploit these theories to the maximum extent, provided that the problem is properly formulated in terms of the objective function(s) and constraints, and the suitable solution method from the optimization theory is identified. Optimization methods are also used in solving and implementing control problems in batch distillation. This section presents design optimization, optimal control, and closed-loop control problems.

Literature on the optimization of the batch column is focused mostly on the solution of optimal control problems, which includes optimizing the indices of performance such as maximum distillate, minimum time, and maximum profit. However, literature on optimal design of batch distillation for performing specified operations by using the constant reflux or variable reflux policies is very limited (Fountain and Husain, 1956; Robinson and Goldman, 1969; Luyben, 1971; Diwekar *et al.*, 1989). This can be attributed to the fact that numerical optimization techniques, such as nonlinear programming (NLP) used in optimal design, are iterative in nature (which requires computational power), while optimal control theory provides analytical expressions (which are difficult to solve). In this section, optimal control problems in the context of performance indices and optimization techniques are described. Some recent articles address the problem of design

and optimal control policy together by combining optimal control theory and numerical optimization methods. This approach for simultaneous optimal design and operation is described later. Closed-loop control of columns is presented at the end of this section.

4.1 Optimal Control Problems

This subsection is devoted to optimal control problems in batch distillation, which have received considerable attention in the literature. In general, control refers to a closed-loop system where the desired operating point is compared to an actual operating point, and knowledge of the error is fed back to the system to drive the actual operating point towards the desired one. However, the optimal control problems we consider here do not fall under this definition of control. Because the decision variables that will result in optimal performance are time-dependent, the control problems described here are referred to as *optimal control problems*. Thus, use of the control function here provides an open-loop control. The dynamic nature of these decision variables makes these problems much more difficult to solve as compared to normal optimization where the decision variables are scalar.

These problems are categorized by (1) performance indices and (2) solution methods. The following subsection discusses the performance indices for optimal control problems, namely maximum distillate, minimum time, and maximum profit, and followed by a subsection on mathematical techniques used to solve optimal control problems, which are calculus of variations, Pontryagin's maximum principle, dynamic programming, and NLP techniques. The first three techniques treat the decision variables as vectors while the NLP approach requires the variables to be transformed into scalars.

4.1.1 Performance Indices for Optimal Control Problems

Optimal control problems can be classified as:

- **Maximum Distillate Problem** – where the amount of distillate of a specified concentration for a specified time is maximized (Converse and Gross, 1963; Kuhl and Brunel, 1971; Murty *et al.*, 1980; Diwekar *et al.*, 1987; Mujtaba and Macchietto, 1988; Logsdon *et al.*, 1990; Farhat *et al.*, 1990; Diwekar, 1992; Logsdon and Biegler, 1993; Meeki and Morari,

1995). This problem can be represented as follows:

$$\begin{aligned} & \text{Maximize} && J = \int_0^T \frac{dD}{dt} dt = \int_0^T \frac{V}{R_1 + 1} dt, \\ & R_1 && \\ & \text{s.t.} && \frac{x_1^1}{dt} = \frac{dB_1}{dt} = \frac{V}{R_1 + 1}, \quad x_0^1 = B_0 - F, \\ & && \frac{dx_2^2}{dt} = \frac{V}{R_1 + 1} \left(\frac{x_0^2 - x_D^2}{B_1} \right), \quad x_0^2 = x_F^2, \\ & && x_{D,avg} = \frac{\int_0^T x_D^2 \frac{V}{R_1 + 1} dt}{\int_0^T \frac{V}{R_1 + 1} dt} = x_D^*, \\ & && 0 \leq t \leq T. \end{aligned} \quad (11)$$

Conover and Gross (1963) were the first to report the maximum distillate problem for binary batch distillation, which was solved using Pontryagin's maximum principle, the dynamic programming method, and the calculus of variations. Diwekar *et al.* (1987) extended this optimization model to multicomponent systems and used the shortcut batch distillation model along with the maximum principle for the calculation of the optimal reflux policy. Logsdon *et al.* (1990) used the orthogonal collocation approach on finite elements and nonlinear programming (NLP) optimization techniques over the shortcut model, and they extended this method to the rigorous batch distillation model (Logsdon and Biegler, 1993) in which they considered the effect of column holdups on optimal control policy. The objective function used by Ezzamel *et al.* (1990) can be classified as a maximum distillate problem although their aim was to maximize production of a specified cut in multifraction operations. In their problem, the batch time for each cut was treated as a decision variable. Linear and exponential approximations to the optimal reflux profiles were implemented, and the NLP optimization technique was applied to obtain the solution. Recently, Meeki and Morari (1995) presented the maximum distillate problem for the middle vessel column and proposed an optimal operating strategy.

• **Minimum Time Problem** – where the batch time needed to produce a prescribed amount of distillate of a specified concentration is minimized.

(Coward, 1966, 1967; Robinson, 1969, 1970; Mayur and Jackson, 1971; Egly *et al.*, 1979; Hansen and Jørgensen, 1986; Christiansen and Jørgensen, 1987; Mujtaba and Macchietto, 1988, 1992; Diwekar, 1992; Bonny *et al.*, 1996; Mujtaba and Macchietto, 1996). Although there are several different formulations for the minimum time problem, Diwekar (1992) derived the following formulations to establish a unified theory for all the optimal control problems:

$$\begin{aligned} & \text{Minimize} && J = \int_0^T dt, \\ & R_1 && \\ & \text{s.t.} && \frac{x_1^1}{dt} = \frac{dB_1}{dt} = \frac{V}{R_1 + 1}, \quad x_0^1 = B_0 - F, \\ & && \frac{dx_2^2}{dt} = \frac{V}{R_1 + 1} \left(\frac{x_0^2 - x_D^2}{B_1} \right), \quad x_0^2 = x_F^2, \\ & && x_{D,avg} = \frac{\int_0^T x_D^2 \frac{V}{R_1 + 1} dt}{\int_0^T \frac{V}{R_1 + 1} dt} = x_D^*, \\ & && 0 \leq t \leq T. \end{aligned} \quad (12)$$

In this objective function, a new dummy variable t^* is introduced as the third state variable (x_3^3) and the relation of t^* with the actual batch time t is given by:

$$\frac{dx_3^3}{dt} = \frac{dt^*}{dt} = 1, \quad t_0^3 = 0. \quad (13)$$

Early approaches to this problem involved solutions of two-point boundary value problems (Coward, 1966, 1967; Robinson, 1969, 1970; Mayur and Jackson, 1971; Egly *et al.*, 1979; Hansen and Jørgensen, 1986; Christiansen and Jørgensen, 1987; Mujtaba and Macchietto (1988) used a piecewise constant reflux policy and a nonlinear programming optimizer to solve this problem. They extended their previous work to the optimal recycle policy for multicomponent systems, which were decomposed to a sequence of pseudo binary optimal control problems (Mujtaba and Macchietto, 1992).

Maximum Profit Problem - where a profit function for a specified concentration of distillate is maximized (Kerthof and Vissers, 1978; Logsdon *et al.*, 1990; Bonny *et al.*, 1999; Li *et al.*, 1997; Mujtaba and Masciella, 1997; Waige and Reklaitis, 1998; Hasebe *et al.*, 1999). Much of the recent research on optimal control problems can be classified into this problem. Kerthof and Vissers (1978) were the first to use the profit function for maximization in batch distillation, and they solved the optimal control problem. The following simple objective function is given by Kerthof and Vissers (1978):

$$\text{Maximize } J = \frac{DP - FC_F}{T + t_s}, \quad (14)$$

$$\text{s.t. } x_{D,avg} = \frac{\int_0^T (1) \frac{y}{R+1} dt}{\int_0^T \frac{y}{R+1} dt} = x_D^*, \quad 0 \leq t \leq T,$$

where P and C_F are cost parameters of product and feed, respectively, and t_s in the denominator is the setup time. However, their objective function did not include the effect of the number of plates and the vapor boil-up rate.

Divekar *et al.* (1987) used a different objective function to solve the profit maximization problem under the constant and variable reflux conditions. Logsdon *et al.* (1990) formulated a new profit function and solved the differential algebraic optimization problem for optimal design and operation. Bonny *et al.* (1999) investigated the optimal design recycling and mixing strategies from the superstructure of batch distillation for maximum profit. Li *et al.* (1997) developed a detailed dynamic multiraction batch distillation model and discretized the model using the orthogonal collocation method on finite elements, and finally solved the maximum profit model using a NLP optimizer. Mujtaba and Masciella (1997) considered a rigorous reactive distillation system for the maximum conversion problem, which can also be classified as the maximum profit problem. The detailed dynamic system is then reduced by using polynomial curve fitting techniques and solved by using a NLP optimizer. Waige and Reklaitis (1998) also considered reactive batch distillation where the objective is to find an optimal campaign structure of

the batch system with or without recycling.

A variant of this objective function is to minimize the mean rate of energy consumption when the market size for the product is fixed by the current demand. The objective function is given by Furukawa *et al.* (1999):

$$\text{Minimize } J = \frac{\int_0^T Q_R(t) dt}{T + t_s} \quad (15)$$

$$\text{s.t. } x_{D,avg} \geq x^*, \quad D \geq D^*,$$

where Q_R is the reboiler heat duty. They used this objective function for optimal control of multivessel columns for the first time. Hasebe *et al.* (1999) also presented the optimal operation policy based on energy consumption for the multivessel column.

4.1.2 Solution Techniques

To solve the optimal control problems, the following four solution techniques have been used in literature. Of these, Pontryagin's maximum principle and nonlinear programming techniques are commonly used nowadays.

- **Calculus of Variations.** The theory of optimization began with the calculus of variations, which is based on the vanishing of the first variation of a functional ($\delta J = 0$) according to the theorem of minimum potential energy which involves the definition of stationary values for a function. This leads to the Euler equation and natural boundary conditions. In batch distillation literature, Converse and Gross (1963) and Murty *et al.* (1980) used this method to solve the maximum distillate problem.

- **Pontryagin's Maximum Principle.** The maximum principle was first proposed in 1956 by Pontryagin and coworkers (Pontryagin, 1956; Bolyanskii *et al.*, 1956). The objective function formulation is represented as a linear function in terms of the final values of a state vector and a vector of constants. Like the calculus of variations, this method is only applicable to optimal control problems for fixed scalar variables. 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.

It is possible to derive the necessary condition for optimality in the calculus of variations from the maximum principle when the decision vector is not constrained. Conversely, by using the technique of the calculus of variations, the weakened form of the maximum principle can be derived.

This principle has been widely used for batch distillation (Converse and Gross, 1963; Coward, 1966, 1967; Robinson, 1969, 1970; Keith and Brunet, 1971; Kerkhof and Visser, 1978; Mayur and Jackson, 1980; Hansen and Jørgensen, 1986; Diweker *et al.*, 1987; Christensen and Jørgensen, 1987).

- **Dynamic Programming.** The method of dynamic programming is based on the *principle of optimality*, as stated by Bellman (1957). In short, the principle of optimality states that the minimum value of a function is a best suitable for multi-stage processes; however, the application of dynamic programming to a continuously operating system leads to a set of nonlinear partial differential equations. This method is used by researchers in solving the batch rectifier (Converse and Gross, 1963; Mandy *et al.*, 1980).

- **NLP Optimization Techniques.** World War II made scientists aware of the usefulness of numerical optimization methods. Numerical optimization techniques involve an iterative scheme. The optimizer invokes the model with a set of decision variables. The model simulates the phenomena and calculates the objective function and constraints, and the information is utilized by the algorithm (optimizer) to find the new set of decision variables. This scheme continues until the optimal decision variables are found. NLP optimization techniques are the numerical tools used for models involving nonlinear algebraic equations. Obviously, applying NLP techniques to optimal control problems involves discretization of the control profile by applying either the orthogonal collocation on finite elements (Agoston *et al.*, 1990; Bonny *et al.*, 1996; Li *et al.*, 1997; Hasebe *et al.*, 1999), the control vector parameterization approach (Charalambides *et al.*, 1995; Mujtaba and Macchietto, 1996; Wajge and Reklaitis, 1998; Furlong *et al.*, 1999), or the polynomial approximation (Mujtaba and Macchietto, 1988; Farhat *et al.*, 1990). These discretization approaches add nonlinearities to the system as the number

of nonlinear equations increase; therefore, they require good initializations and may result in sub-optimal solutions. On the other hand, the polynomial approximation methods depend on the crucial decision of choosing the right type and order of polynomials for the control profile approximation.

A new approach to optimal control problems in batch distillation, proposed in a paper by Diweker (1992), combines the maximum principle and the NLP techniques. This algorithm reduces the dimensionality of the problem (caused by NLP techniques) and avoids the solution of the two-point boundary value problems (caused by the maximum principle). Furthermore, it was shown that for batch distillation problems, bounds could be imposed on the control vector by virtue of the nature of the formulation.

4.2 Closed-Loop Control

The two traditional batch operation policies, constant reflux and variable reflux policies, involve different control strategies. For the constant reflux policy where the distillate composition is continuously changing, the average distillate composition can only be known at the end of operation unless proper feedback from the operation is obtained. The control of the average distillate composition is, then, of an open-loop control nature. However, the variable reflux policy is inherently a feedback operation because the reflux ratio is constantly adjusted to keep the distillate composition constant. The purpose of the designing of a closed-loop control scheme is to reduce the sensitivity of the plant to external disturbances. Since batch distillation starts with total reflux to obtain steady state and the distillate is withdrawn after that point, the reflux ratio and distillate composition may oscillate if a controller gain is not properly selected. This is the reason the constant composition control proves to be very challenging. This subsection describes recent research efforts on the closed-loop control problems.

Quintero-Marmol *et al.* (1991) and Quintero-Marmol and Luyben (1992) proposed and compared several methods for estimating the on-line distillate composition by the feedback control under the constant reflux operating policy in a batch rectifier. An extended Luenberger observer for tracking the distillate composition profile was proved to provide the best result.

Bosley and Edgar (1992) considered modeling, control, and optimization aspects of batch rectification using nonlinear model predictive control

(NMPC), and implemented an optimal batch distillation policy that was determined *a priori* by the off-line optimization. NMPC can determine the set of control moves, which yield the optimal trajectory and allow explicit constraints on inputs, outputs, and plant states. It is known that NMPC is one of the best approaches for distillate composition control; however, the control scheme is computationally intensive because optimization problems are solved inside this control loop. This work was further studied by Finetock *et al.* (1994) who studied nonideal binary batch distillation under the variable reflux operating policy. Since the gain space can be changed significantly after a switch to the production phase, they suggested a gain-scheduled PI controller based on NMPC if the instantaneous distillate composition is known. Filici *et al.* (2000) also considered NMPC as well as PAD (programmable adaptive controller) and STR (self-tuning regulator) for optimization and on-line operation, and suggested that NMPC be generally applicable in any feed mixture conditions.

Besides NMPC, Barolo and Berio (1998) provided a framework for obtaining composition control in batch distillation using a nonlinear internal model control (NIMC) approach. NIMC, proposed by Henson and Seborg (1991), can exactly linearize the system input-output map and be easily tuned by using a single parameter for each component. The distillate composition is estimated by the selected temperature measurements. They also used an extended Luenberger observer for a composition estimator. Although this approach can be reliable and easily implemented, the authors pointed out the problem of selecting the best temperature measurement locations and the problems with using the extended Luenberger observer in case of a large number of trays of a batch column. For a tighter composition control, more research is necessary to develop a robust and fast closed-loop control scheme.

Closed-loop control schemes have also been applied to new column configurations and complex batch systems. Sorensen and Skogestad (1994a) presented control schemes for the batch stripper. For the control of the middle vessel column, Barolo *et al.* (1996) first proposed and examined several control schemes with or without product recycling. They showed the experimental results of the proposed control structures for dual composition control with or without impurity. Farsicman and Diwekar (1998) proposed dual composition control in which the two composition control loops can be decoupled if the instantaneous product compositions are known. The degree of interaction between the two composition control loops can be assessed using the relative gain array technique. Phinister and Scider (2000) extended

the two composition control loops to continuous distillation having a middle vessel in order to overcome the common problems in the dual composition control of continuous distillation.

Hastbe *et al.* (1995) proposed a single loop cascade control system to control the composition of each vessel in the multivessel column. The vessel holding under total reflux is the manipulated variable, and the reflux flow rate from each vessel is, then, controlled by a simple PI controller. Wittgens *et al.* (1996) and Skogestad *et al.* (1997) developed a simple feedback control strategy in which the temperature at the intermediate vessel was controlled by the reflux rates from the vessels, thereby adjusting the vessel holdups indirectly. Further, Furlonge *et al.* (1999) compared different control schemes, including optimal control problems in terms of energy consumption.

The feedback control in the extractive batch distillation has appeared little in literature. Sorensen *et al.* (1996) proposed a control scheme to track the optimal temperature profile determined *a priori* by using a conventional PI temperature controller. Monroy-Lopera and Alvarez-Ramirez (2000) extended Barolo and Berio (1998)'s work to reactive batch distillation in which an input-output linearized feedback is proposed.

Future works in the closed-loop control problems can involve locating the proper temperature measurement locations, easy parameter tuning, and/or focusing on tracking the optimal profiles, as well as the 'on-spec' products.

5 EMERGING BATCH COLUMNS, COMPLEX SYSTEMS, AND SYNTHESIS

In the previous sections, we described different aspects of batch distillation including the development of a hierarchy of models ranging from simplified to rigorous, optimization, and optimal control of the batch distillation operation. This section presents discussion on alternative emerging column configurations, and thermodynamically or kinetically complicated batch distillation systems such as azeotropic, extractive, and reactive distillations. In addition, this section describes how these complex batch column configurations and/or complex systems result in difficult batch distillation synthesis problems.

5.1 Emerging Batch Columns

In the introduction, Figure 3 showed the off-cut recycling column (Figure 3c), batch stripper (Figure 3d), middle vessel column (Figure 3e) and multivessel column (Figure 3f) configurations as emerging batch columns. These columns are described here.

5.1.1 Off-cut Recycling Batch Distillation

Research on the design and optimization of this operation has mainly involved the performance evaluation like minimum batch time and/or waste amounts based on the degree of difficulty of separation, mixing and recycling strategies.

Mayor *et al.* (1970) suggested an off-cut recycling or periodic operation in which the fresh feed of each charge is mixed with the recycled off-cut products from the previous charge. Unlike simple batch distillation, batch distillation with recycled waste cut consists of two steps, and hence a quasi-steady state of operation can be assumed when the number of batches increases. They observed a 5% reduction in the batch time for the binary system with a recycled cut. Christensen and Jørgensen (1987) solved the minimum time problem of this operation by using Pontryagin's maximum principle and the orthogonal collocation method. Their computational results showed that off-cut recycling may lead to significant time savings for difficult separation systems ($g > 0.75$) compared to batch distillation without off-cut recycling. The degree of the difficulty of separation (g) is the ratio of the necessary N_{min} in the column at total reflux and constant product composition to the actual number of ideal trays in the given column. Besides g , a capacity factor that is the total on-specification products divided by the total batch time was used to evaluate different off-cut recycling strategies for multicomponent batch distillation with off-cut recycling (Quintero-Marmol and Luyben, 1990). They suggested to perform individual binary batch distillation on each off-cut, resulting in 30 ~ 40 % increases in the capacity factor.

Optimization and optimal control theories have also been applied to batch distillation with off-cut recycling (Mujalaba and Marchetto, 1992; Marchetto and Mujalaba, 1996; Bonny *et al.*, 1996). Mujalaba and Marchetto (1992) proposed an optimal recycle policy for multicomponent batch distillation using the NLP technique for the minimum time problem based on a quasi-steady state batch distillation model (which was finally decomposed to a

pseudo binary batch model). The results showed significant savings in batch time and improvements in productivity for a moderate degree of difficulty of separation cases ($0.4 < g < 0.6$). However, their model based on the assumption of sharp separation becomes invalid when g is greater than 0.6. They extended this work to the determination of the optimal recycling of the off-cuts by the multiperiod reflux optimization technique (Marchetto and Mujalaba, 1996), in which CVP (control vector parameterization) was used to discretize the reflux profile over different periods. Bonny *et al.* (1996) provided optimal strategies for a batch distillation campaign, where the main interested strategies were the optimal determination of the mixing strategy and the stop-cut recycling strategy. Among their general suggestions, fixed constant reflux ratio per batch was observed as a good strategy for the examples considered.

As described earlier, Zamer *et al.* (1998) derived a shortcut model for multiple task batch distillations with or without the off-cut recycling using a partition function where the actual composition profiles are approximated by the profiles at the total reflux condition. Waige and Reklaitis (1998) developed a general optimal campaign structure (campaign optimization) for reactive batch distillation with waste cuts. The optimal policies were obtained by multiperiod reflux optimization with a CVP discretization and a NLP technique.

5.1.2 Batch Stripper

Although the batch stripper, often called an inverted batch column, originally proposed by Robinson and Gilliland (1950), is not a true emerging batch column, it has gained much attention in recent literature. In this column configuration the feed mixture is charged into the top reflux drum, and the products are withdrawn at the bottom reboiler.

Benot *et al.* (1991) developed a semi-rigorous model of the batch stripper for multicomponent azeotropic distillation and showed that the batch stripper, compared to the rectifier, is essential to break a minimum boiling point azeotrope. Svendsen and Skogestad (1996) compared the batch stripper with the batch rectifier in terms of batch time and proposed that the inverted column configuration is better than the regular column for separations where the light component in the feed is present in a small amount. They also reported that in some cases the stripper can separate feed mixtures while the rectifier design is infeasible for that separation. Lotter and Diwekar (1997) published a shortcut model for the stripper based on the FUG method, and

Kim and Diwekar (2000), based on this shortcut model, derived more generalized heuristics for column selection using various performance indices, namely product purity and yield, feasibility and flexibility, and thermodynamic efficiency.

5.1.3 Middle Vessel Column

This column configuration consists of a middle vessel between two sections of the batch column. The feed is initially charged into the middle vessel, and the products are simultaneously withdrawn from the top and the bottom of the column. The middle vessel column can be an ideal configuration for ternary batch systems.

Robinson and Gilliland (1950), Bortoloti and Guarise (1970), and Deyvadh and Chutchev (1976) were the earlier researchers who mentioned the possibility of this column configuration. However, only recently, analysis of this column configuration has been published in the 1990s (Hasebe *et al.*, 1992; Davidyan *et al.*, 1994; Mujtaba and Macchietto, 1994; Meeki and Morari, 1995; Barolo *et al.*, 1996; Lotter and Diwekar, 1997).

Hasebe *et al.* (1992) configured a heat-integrated middle vessel column and proposed that the middle vessel column is more effective in separating ternary components than the rectifier. In their study, the column was operated in such a way that the light impurity was taken off the top and the heavy impurity was removed from the bottom. This operation is sustained until the desired product specification is reached in the middle vessel.

Davidyan *et al.* (1994), based on their previous works (Davidyan *et al.*, 1991a,b,c), analyzed the dynamic behavior of the middle vessel column for ideal binary and ternary, and azeotropic ternary systems. They found additional steady states, which are stable or unstable singular points of a dynamic system describing the column. They also introduced a new parameter q' ; which is the ratio of the vapor boilup rate in the rectifying section to the vapor boilup rate in the stripping section. Depending on the value of the variable q' , the column shows a qualitatively different behavior for a domain of the reflux and reboil ratio. Figure 7 shows the effect of q' on the top and bottom product purities. For $q' = 1$, the distillate composition of the more volatile component increases with time, and this is a favorable trend for the light key distillate. However, the bottom composition of the least volatile component is decreasing. These trends are opposite to those of batch rectification whose trends are similar to the case of $q' = 10$. Therefore, the new degree of freedom q' is an important parameter to be used in optimizing

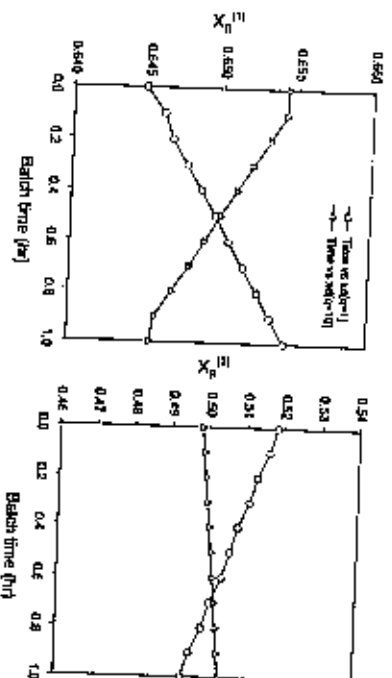


Fig. 7: The effect of q' on the top and bottom product purities in the middle vessel column.

the operation. Meeki and Morari (1995) extended their previous work under the infinite separation and the minimum reflux conditions and proposed that the middle vessel column always outperforms than the rectifier and the stripper in terms of batch time. For a binary separation system, they also found that the steady-state operation corresponding to $q' = 1$ is the optimal control policy.

Besides column dynamics, this column configuration was also applied to reactive batch distillation by Mujtaba and Macchietto (1994). Lotter and Diwekar (1997) developed the shortcut model and derived feasibility criteria for the middle vessel design. Barolo *et al.* (1996) proposed several control schemes for this column configuration and experimentally validated the dual control system for this column configuration. The dual control system was also studied by Farschman and Diwekar (1998) and Pflüster and Seider (2000).

This column configuration is very flexible and effective, and hence one can, in theory, simultaneously obtain very pure components in the top, bottom, and middle vessel. For example, Sarfir *et al.* (1995) investigated extractive distillation in the middle vessel column and found that this column can recover all of the pure distillate product from an azeotropic feed with a relatively small size of reboiler, while a rectifier alone would require a still pot of infinite size.

5.1.4 Multivessel Column

Hasebe *et al.* (1995) presented a heat integrated multi-effect batch distillation system (MIBDS) as an alternative to continuous distillation. The feed was initially distributed among all the middle vessels and operated at the total reflux policy. They proposed a composition control system in which the vessel holdups are manipulated by level controllers. They concluded that this new emerging column configuration can have better separation performance than continuous distillation for systems having a larger number of products. Hasebe *et al.* (1997) published an optimal operation policy for this column using variable holdup modes. They optimized the liquid flow rates in order to minimize the batch time and concluded that the varying holdup mode resulted in up to 43% more distillate than that of the constant holdup mode. Recently, Hasebe *et al.* (1999) optimized the holdup of each vessel as a function of time for the total reflux multivessel systems. They also compared the optimal policy with the constant reflux and variable reflux policies, where the variable reflux policy for a ternary system is 18 ~ 38 % greater in performance index, defined as the amount of products per batch per total batch time.

Skogestad *et al.* (1997), based on their previous work (Wijffens *et al.*, 1996), reported a new column configuration called a multivessel column. This column is operated at total reflux condition. They showed that the steady-state compositions in the intermediate vessels could be maintained regardless of the initial feed composition by controlling the liquid rate from the middle vessel so that the temperature of the tray just below the middle vessel remained constant. This operation policy can be the ideal operation policy of batch distillation, especially for the middle vessel and multivessel column. The total reflux mode is commonly used for the multivessel column (Skogestad *et al.*, 1997) because multiple products can be accumulated in each vessel according to their relative volatilities. As a variant of this operating mode, the cyclic operation mode has also been studied. Some literature can be found on the cyclic operation policy (Garb and Holland, 1967; Block, 1967; Gonzalez-Vlasco *et al.*, 1987; Nowicki and Górak, 1988; Sørensen and Skogestad, 1994b), which is essentially a variant of total reflux condition. Recently, Sørensen (1999) presented a comprehensive study on the optimal operation of the cyclic operating policy of the batch rectifier, stripper, and middle vessel columns. The computational result and experiments showed a significant savings in batch time for some separations. Furuta *et al.* (1999) extended their previous study to optimal control

problems and developed more detailed rigorous equations with dynamic energy balance equations, liquid and vapor holdups, and dry and wet head losses on each tray. They compared various operating policies in terms of a mean energy consumption rate. They found that the optimal initial feed distribution greatly improves the column performance, resulting in an energy consumption rate half that of the rectifier.

5.2 Complex Batch Distillation Systems

Thermodynamically and kinetically complex systems like azeotropic, extractive, and reactive systems pose additional bottlenecks in design and operation of batch columns. The operational flexibility offered by batch distillation, along with the new emerging designs, can provide promising alternatives for circumventing the bottlenecks. The following sections describe the methods for analyzing these complex systems. These methods also provide heuristics for synthesis of these columns especially in terms of the different cuts obtained in a single column or performance comparison of the complex columns.

5.2.1 Azeotropic Batch Distillation

Azeotropic distillation is an important and widely used separation technique as a large number of azeotropic mixtures are of great industrial importance. Despite their importance, azeotropic distillation techniques remain poorly understood from a design standpoint. This is because of the complex thermodynamic behavior of the system. Theoretical studies on azeotropic distillation have mainly centered around methods for predicting the vapor-liquid equilibrium data from liquid solution models and their application to distillation design (vanDongen and Doherty, 1985b). However, only during the past two decades has there been a concerted effort to understand the nature of the composition region boundaries. Doherty and coworkers (Doherty and Perkins, 1977, 1978a,b, 1979; vanDongen and Doherty, 1985b; Foucher *et al.*, 1991; Bernat *et al.*, 1990, 1991) in their pioneering works proposed several new concepts in azeotropic distillation. They established the use of ternary diagrams and residue curve maps in the design and synthesis of azeotropic continuous distillation columns. In batch distillation, they outlined a synthesis procedure based on the residue curve maps.

The residue curve map graphs the liquid composition paths that are

solutions to the following set of ordinary differential equations:

$$\frac{dx_i}{dt} = x_i - y_i; \quad i = 1, 2, \dots, n-1 \quad (16)$$

where n is the number of components in the system, and the independent variable, warped time (ξ), is a monotonically increasing quantity related to real time. One can see that Equation 16 is one form of the Rayleigh equation described earlier. The residue curve map occupies a significant place in the conceptual design stage of column sequencing in continuous distillation, and fractions (cuts) sequencing in batch distillation (Bernot *et al.*, 1990, 1991; Ahmad *et al.*, 1998).

Bernot *et al.* (1990, 1991) presented the general behavior of ternary azeotropic distillation and compared the batch rectifier and stripper for the minimum boiling azeotropic system. They suggested the use of the batch stripper to break the azeotropic. Espinosa and Salomone (1999) developed a modified shortcut model of batch rectification for nonideal azeotropic systems. Their model, based on the constant minimum reflux ratio, estimated the instantaneous separation performance from the geometry of the internal profiles, thus not requiring stage-to-stage computation. Analysis of the azeotropic distillation in the middle vessel column was presented by Cheong and Barton (1999). The assumptions underlying this analysis were an infinite number of trays and infinite reflux and infinite reboil ratios. The top and bottom products are governed by the concept of steering the middle vessel composition (x_M), which is the vector cone of possible motion for the middle vessel composition. The vector is analyzed in terms of the dimensionless middle vessel parameter (λ), where

$$\lambda = \frac{D}{D+B} \quad (17)$$

This λ is related to q' as defined earlier. By varying λ (i.e., changing the production rates), it is possible to cross the middle vessel boundaries and thus overcome distillation barriers. One way of steering the middle vessel composition using λ is shown in Figure 8.

Despite the advances in the thermodynamics for predicting azeotropic mixtures, feasible distillation boundaries, and sequence of cuts, the

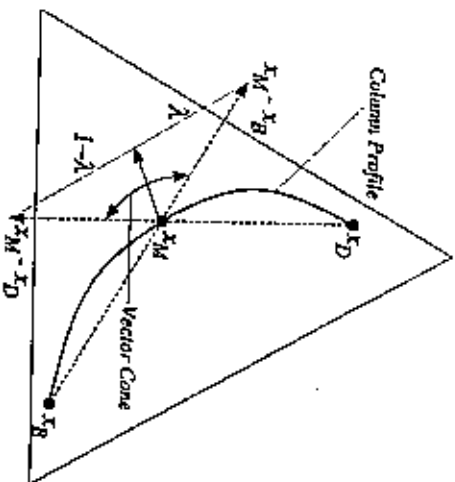


Fig. 8: One way of steering the middle vessel composition where λ is a dimensionless middle vessel parameter (Reproduced from Cheong and Barton, 1999).

azeotropic batch distillation system is still incipient in terms of design, optimization, and optimal control.

5.2.2 Extractive Batch Distillation

Extractive batch distillation can provide advantages of both batch distillation and extractive distillation, and thus this process can be very useful for separation and recovery of waste solvent streams that generally form multicomponent azeotropes. However, most of the recent research efforts on this kind of distillation is limited to feasibility analysis.

Yadav *et al.* (1993) first developed a dynamic simulation model of the extractive batch rectification process with continuous feeding of an entrainer, and validated the model experimentally. The extractive distillation process using the rectifier consists of four steps which are: (1) operation under total reflux without solvent-feeding, (2) operation under total reflux with solvent feeding, (3) operation under finite reflux with solvent feeding, and (4) operation under finite reflux without solvent feeding.

However, the operation steps and the sizes of the reboiler can be reduced if

the middle vessel column is used. Safrit *et al.* (1995) and Safrit and Weisenberg (1997) investigated batch extractive distillation in the middle vessel column. They showed that the extractive process is comprised of two steps (Operations 2 and 3) and requires a much smaller still pot size. They also identified feasible and infeasible regions, and showed that by varying column conditions such as the product rate, reflux ratio, and reboil ratio, one can 'steer' the middle vessel composition to escape from an infeasible region if it is located in one. The concept of steering is also used by Cirrong and Barton (1999) as described in the previous subsection.

Safrit *et al.* (1995) also showed that the middle vessel column can theoretically separate mixtures into their pure states. But from the extensive study on feasibility of extractive batch distillation by Leites *et al.* (1998), a theoretical recovery of 100 percent can only be possible when the steering is toward the simplex of the intermediate component on the triangular diagram. The authors found that the necessary and sufficient condition for feasibility is to have at least one connecting route between the still path and the rectifying profile. It is the extractive profile that connects the profiles (Figure 9). By varying the ratio of the entrainer flow rate to the vapor flow rate (E/V), one can change the extractive profile and thus find feasible operating conditions. It should be remembered that since this feasibility analysis is based on the

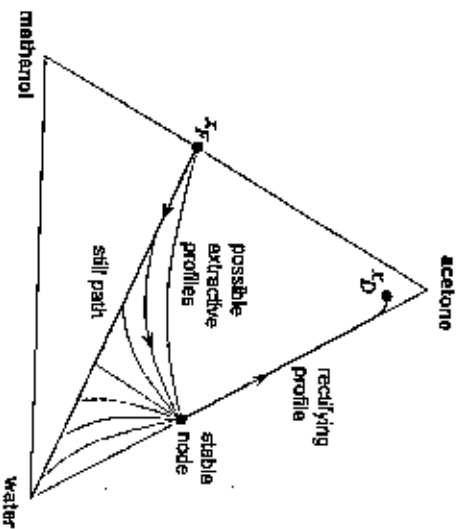


Fig. 9: Possible extractive profiles for a feasible operation in Step 2.

batch rectifier, not the middle vessel column, it also requires four steps and may require a large-sized reboiler.

5.2.3 Reactive Batch Distillation

Although reactive distillation was acknowledged as a unit operation as early as in the 1920s, it has gained its research interest as an excellent alternative to both reaction and separation since the 1980s. For example, most of the new commercial processes of MTBE (methyl-*t*-butyl ether, an anti-knocking agent) are based on continuous reactive distillation technologies.

The analysis of a reactive batch distillation model in a staged column was first published by Cullis and Reklaitis (1986). Using a stiff integrator for the differential and algebraic equations, they presented a numerical solution technique for the esterification of 1-propanol and acetic acid. Albert *et al.* (1991) and Sorensen *et al.* (1996) developed control schemes for reactive batch distillation using repeated simulation techniques. The use of the middle vessel column for reactive distillation was studied by Mujtaba and Macchietto (1994).

Wigge *et al.* (1997) developed a new solution technique based on the orthogonal collocation method on the finite element method for the reactive batch distillation of a packed column. The differential reactor model of a packed column, originally designed by Hinch and Rousseau (1988), was then reduced to the low-order polynomials with desired accuracy. They compared the results with those from the finite difference method and global collocation method for non-reactive packed-bed batch distillation systems, and showed that their approach was more efficient. Wigge and Reklaitis (1998) extended their previous work to the optimal campaign structure for reactive batch distillation, which can offer reasonably sharp separations between successive cuts and reduce the amount of waste off-cuts. To obtain the optimal reflux policies or profiles for the maximum distillate or minimum time problem, multiperiod reflux optimization (Macchietto and Mujtaba, 1996) can be applied. They showed that for the same production rate, the waste generation can be significantly reduced under the optimal campaign structure.

An efficient optimization approach for reactive batch distillation using polynomial curve fitting techniques was presented by Mujtaba and Macchietto (1997). After finding the optimal solution of the maximum conversion problem, polynomial curve fitting techniques were applied over these solutions, resulting in a nonlinear algebraic maximum profit problem

that can be efficiently solved by a standard NLP technique. Four parameters in the profit function, which are maximum conversion, optimum distillate, optimum reflux ratio, and total reboiler heat load, were then represented by polynomials in terms of batch time. This algebraic representation of the optimal solution can be used for on-line optimization of batch distillation.

Veniaminova *et al.* (1999) developed a semi-rigorous model for a reactive distillation system forming multiple azeotropes. They constructed the model equations using two dimensionless parameters, warped time (S) and Damköhler number (Da), and introduced a distillation strategy of removing the aqueous phase in the condenser as a distillate. They also derived an explicit expression for the reflux policy for a special case of zero sum of reaction coefficients.

A dynamic rate-based model for packed-bed batch distillation was recently presented (Kreul *et al.*, 1998, 1999), in which a solid catalyst was used first in the reactive batch distillation modeling. The pilot-scale experiments were conducted with strong anion-exchange resins. The results were compared with the experimental data and with the results from its counterpart, the equilibrium-based model. The rate-based model provides more accuracy, much higher physical significance, and more predictability of the experimental data even though the formulation of the rate-based model is complicated.

Since reactive batch distillation is normally carried out in a packed-bed batch distillation column, the following paragraphs are devoted to designing of packed-bed batch columns.

Packed-bed batch distillation, with or without reactions, is a very effective method for separating specialty chemicals by flexibility and cost as compared to staged batch columns (Srivastava and Joseph, 1984). In general, there are two solution techniques: heat and mass transfer model (rate-based model or differential contact model) and non-equilibrium stage model (Gross *et al.*, 1990). The first method is based on the mass and heat balances of a differential element of the packing while the second is based on the actual finite layer of packing, resulting in nonlinear algebraic equations. Both methods can ideally provide the same results, but the solution efficiency is quite different. Most of the recent literature on packed-bed batch distillation exploits the mass and heat transfer model.

Felhan *et al.* (1982) developed a generalized model for packed columns, which included nonlinear VLE, axial dispersion, and energy balances, and they validated their model with experiments. The model was solved by the

finite difference method, which had stability problems when integrating the system equations. The model was further investigated by Aly *et al.* (1987) with a steady-state model under total reflux with axial and radial dispersion. This steady-state model was then applied by the finite element method of the Galerkin-type for rapid convergence. However, the Galerkin method is hard to implement in machine computing. Christensen and Jørgensen (1987) presented numerical techniques to simulate packed columns in which the orthogonal collocation method was applied to solve the minimum time problem.

As described earlier, most of the recent studies on reactive batch distillation use packed-bed batch columns, and thus some of them are briefly mentioned here. Mujtaba and Machiello (1994) presented a comprehensive study of the optimal operation of reactive batch distillation in the middle vessel column. Weige *et al.* (1997) and Weige and Reklaitis (1998) applied the orthogonal collocation over the finite elements for the differential contactor model of reactive batch distillation. A dynamic rate-based model for packed-bed batch distillation was recently presented (Kreul *et al.*, 1998, 1999).

5.3 Batch Distillation Synthesis

The complexity in batch distillation design and operation is also reflected in the batch distillation synthesis problem. In the continuous distillation, optimal column sequencing is the main focus of synthesis research. Several past reviews are available on this subject (Stephanopoulos, 1980; Nishida *et al.*, 1981; Grossmann, 1990). Unlike continuous distillation synthesis, the area of batch distillation synthesis is complicated by the transient nature. Decisions like cut selection, operating mode, configuration type, and column sequencing enter into the synthesis problem. For complex systems like azeotropic, extractive, and reactive distillation, identifying the region boundaries and steering towards feasible and optimal regions add further complications to the problem. However, as seen in the previous section, the theoretical and geometric analysis can provide right directions towards the optimal synthesis problem in this area (Bernot *et al.*, 1990, 1991; Caocong and Barton, 1999).

The state of the art techniques used in the solution of synthesis problems include: (1) the heuristic approach which relies on intuition and engineering knowledge, (2) the physical insight approach which is based on exploiting

basic physical principles, and (3) the optimization approach. In this article two common approaches, heuristics and optimization, are discussed.

The recent literature in batch distillation has been devoted to comparing emerging column configurations with the conventional one, thereby obtaining heuristics for optimal column configuration, optimal design, and optimal operating conditions (Chisti and Ibraheem, 1991; Meshi and Morari, 1995; Hasebe *et al.*, 1995; Sørensen and Skogestad, 1996; Kim and Diwekar, 2000). In these studies, parameters such as product purity, batch time, or total cost were evaluated to compare the performance of column configurations. Choffit and Ibraheem (1991) compared the rectifier with the stripper in terms of annual cost and product purity. They noted that the rectifier is better for the more volatile component products while it is more economical to obtain less volatile component products using the stripper. Meshi and Morari (1995) compared three column configurations in terms of the batch time under fixed product purity and infinite number of plates. It was observed that the middle vessel column always has the shortest batch time, and the rectifier is the next. Sørensen and Skogestad (1996) studied two competing column configurations, rectifier and stripper, in the context of minimum optimal operating time, and also provided the dynamic behavior of these columns. They concluded that the stripper is the preferred column configuration when a small amount of the more volatile component is in the feed, and that the rectifier is better when the feed has a high amount of the more volatile component. Although several studies support the same heuristics, there are also studies which present contradictions between suggested heuristics. For example batch time studies of Meshi and Morari (1995) and Sørensen and Skogestad (1996) give a conflicting result with respect to feed composition. This is due to limited ranges of parameters and systems considered as well as the complexity and difficulty of the problem of column selection.

In order to elicit comprehensive heuristics, the analysis must cover a wider range of column configurations, operation policies, and design variables, and various performance indices need to be included. Kim and Diwekar (2000) extended the column configuration problem using four performance indices: product purity, yield, design feasibility and flexibility, and thermodynamic efficiency. It is generally observed that the rectifier is a promising column configuration for the more volatile component product, and that the stripper is better in the opposite case. Feasibility studies based on the minimum number of plates and the minimum reflux ratio showed whether such a high purity configuration is flexible for changing operating conditions.

It is found that the rectifier and the stripper have distinctive feasibility regions in terms of the feed composition. Thermodynamic efficiency indicates how close a process or system is to its ultimate performance and also suggests whether the process or system can be improved or not. The rectifier can also be a promising column configuration in terms of thermodynamic efficiency, but in some conditions, higher efficiencies of the stripper or the middle vessel column are observed. Furthermore, for the middle vessel column, the thermodynamic efficiency is greatly affected by an added degree of freedom (4th). This systematic and parametric study concludes that the trade-off between performance indices should be presented as a multi-objective framework.

5.4 Computer Aided Design Software

It is difficult to analyze batch distillation without using computers due to the two reasons stated before: (1) the process is time varying, and one has to resort to complex numerical integration techniques and different simulation models for obtaining the transients, and (2) this ever-changing process also provides flexibility in operating and configuring the column in numerous ways. Based on the current state of the art in batch distillation techniques and computer simulation technology, Table 3 identifies the required functionality and the rationale behind it.

There are several commercial software packages for simulations, optimizations, and/or optimal controls of batch distillation. These include Bdist-SimOPT (Batch Process Technologies), BatchSim (Simulation Sciences), BatchFrac (Aspen Technology, based on Boston *et al.* (1983)), and MultiBatchDS (Batch Process Research Company). Bdist-SimOPT and MultiBatchDS are derived from the academic package BATCHDIST (Diwekar and Madhavan, 1991). Most of these packages except MultiBatchDS are usually limited to conventional systems as they were developed in early or late 80s.

Table 3
Batch distillation software requirements.

Features	Why
Windows	User friendly state of the art input/output interface
Databank	Ability to generate data from structural information
Operations	
	Constant reflux
	Variable reflux
	Fixed eqn. Optimal
	Optimal reflux
Models	
	Shortcut
	Semi-rigorous
Options	Hierarchy of models for numerical stability, design feasibility, and advanced system designs
	Design feasibility
	Optimization
	Reactive distillation
	Three-phase distillation
	Uncertainty analysis
Configurations	
	Semi-batch
	Recycle waste cut
	Rectifier
	Stripper
	Middle vessel column
	Emerging designs provide promising directions for effective designs to obtain purer products

6 CONCLUSIONS

This paper presented a complete review of batch distillation literature starting from the first theoretical analysis to the current state of the art in computer aided design and optimization methods. The new advances in batch distillation include novel column configurations, optimal designs, optimal operation policies, and new methods of analysis. These new advances can increase the possibility of using batch distillation profitably for a wide variety of separations, but they also present bewildering problems of selection of the proper configuration, the right operating mode, and optimal design parameters. Thus, we will certainly see future researchers working on various aspects of design, analysis, and synthesis of batch distillation, some of which are outlined below.

- A more extensive analysis for each column configuration must be carried out. For example, the effect of σ' on the performance of the middle vessel column has not been fully investigated. For the multivessel column, no general guidelines or heuristics exist for column holdups and operating modes because of the additional degrees of freedom.
- Azeotropic, extractive, and reactive distillations and off-cut recycling operations have been studied extensively in recent years, but they are in the developing stage. For instance, while in continuous reactive distillation, solid catalysts are commonly used, but there are only a few applications of solid catalysts in batch reactive distillation in theory and practice.
- Comprehensive heuristics for optimal design and synthesis should be derived. Several heuristics and trade-offs between heuristics can be found, but they are still limited to the systems considered.
- Batch processes often encounter feed composition variations and other operational uncertainties. Consideration of uncertainties at various stages of design and operation can provide useful and cost effective solutions to the batch processing industries.
- One of the important research areas in this field is batch distillation synthesis. Based on future advances in batch distillation, batch distillation synthesis from a superstructure can lead to the most promising and flexible column configuration with the right operation policy and conditions.

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Reviews in Chemical Engineering

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NOTATION

α	relative volatility
B	amount of bottom residue [mol]
$\frac{dB}{dt}$	bottom product flow rate or change of bottom product [mol/hr]
C_D	cost of distillate [\$/mol]
C_F	cost of feed [\$/mol]
C_H	cost of heating medium [\$/mol]
D	amount of distillate [mol]
$\frac{dD}{dt}$	distillate rate [mol/hr]
ξ	entrainer feed rate [mol/hr]
F	amount of feed [mol]
H_j	molar holdup on plate j [mol]
H_0, H_D	condenser holdup [mol]
h_n	enthalpy of the liquid in the condenser [J/mol]
h_j	enthalpy of the liquid stream leaving plate j [J/mol]
h_j	enthalpy of the vapor stream leaving plate j [J/mol]
L_j	liquid stream leaving plate j [mol/hr]
l_0	liquid reflux at the top of the column [mol/hr]
n	number of components
N	number of plates
N_0	number of plates in the bottom section of a column
N_T	number of plates in the top section of a column
P_r	sales value of the product
q	degree of difficulty of separation (the ratio of the necessary N_{min} in the column at total reflux and constant product composition to the actual number of ideal trays in the given column)
q'	ratio of the top vapor flow rate to the bottom vapor flow rate
Q_R	reboiler heat duty
R	reflux ratio (= L/D)

R_f	reflux ratio as a function of time
T	batch time [hr]
t_s	setup time for each batch [hr]
V_j	vapor stream leaving plate j [mol/hr]
x	liquid-phase mole fraction
x_D	liquid-phase mole fraction of the distillate
$x_{D,av}$	average distillate mole fraction
x_F	liquid-phase mole fraction of the feed
x_M	liquid-phase mole fraction of the middle vessel still
x_1	state variable at time t representing quantity of charge remaining in the still, B_t [mol]
x_2	state variable representing the composition of the key component in the still at time t , $x_B^{(1)}$
y	vapor-phase mole fraction

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Ki-foo Kim and Urmila M. Divekar

Reviews in Chemical Engineering

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