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Batch distillation simulation using the quasi-state column approximation

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**BATCH DISTILLATION SIMULATION USING
THE QUASI-STEADY-STATE COLUMN APPROXIMATION**

A Thesis

Presented to

The Faculty of the Department of Chemical Engineering

San Jose State University

In Partial Fulfillment

of the Requirements for the Degree

Master of Science

by

Keith A. Friedman

December 1995

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ABSTRACT

BATCH DISTILLATION SIMULATION USING THE QUASI-STEADY-STATE COLUMN APPROXIMATION

by Keith A. Friedman

Since the 1960's, batch distillation column design has been aided by computer solution of rigorous fully-dynamic process models. Recently, researchers have substantially increased the speed of batch distillation simulation through the use of the quasi-steady-state column approximation (QSSCA) approach. This approximation says that the transient behavior of the column can be neglected relative to transients in the boiler, when the material holdup in the column is much smaller than that in the boiler.

Despite its advantages and successes, batch distillation simulation using the QSSCA approach is not readily available to working chemical engineers using common flowsheet simulators. Therefore, the QSSCA approach to batch distillation simulation was implemented and investigated on a prototypical process simulator, ASPEN PLUS. The implementation is presented and illustrated with examples. It was tested on published case studies of batch distillation. The results compare favorably with experimental data and other simulations.

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CHAPTER 1. INTRODUCTION

Since the 1960's, computers have aided the design of batch distillation columns by solving rigorous, fully dynamic (RFD) process models. Recently, researchers have substantially increased the speed of batch distillation simulations with the quasi-steady-state column approximation (QSSCA) approach. This thesis pursues this research by investigating a particularly advantageous implementation of the QSSCA approach.

This chapter introduces and outlines this work. To justify the effort, the first section describes the importance of batch distillation and the need for process simulation. The second section surveys modern methods of batch distillation simulation, including the RFD and QSSCA approaches. This survey reveals an important direction for extension of the state-of-the-art: implementation of the QSSCA approach on a general-purpose process simulator (GPPS). This is the objective of this thesis. The third section presents the primary research objective and corresponding hypotheses associated with this investigation. Besides investigating a simulation approach, this work has other implicit benefits that are described in the fourth section of this chapter.

1.1 Batch Distillation Review

Dictionaries (Lapedes, 1978; Mish, 1983) define distillation as a process of applying heat and boiling a liquid mixture, and then condensing the vapor to progressively separate the mixture components by differences in their volatilities.

Distillation is also known as fractionation or rectification, and distillation columns are also called towers or stills. Distillation can be continuous, with continuous feed to a column whose conditions are steady-state. Alternatively, it can be discontinuous, with a batch of feed loaded into the boiler at the beginning and column conditions changing as distillation proceeds.

Continuous or discontinuous, distillation is a superior separation process.

In his book Separation Processes, C. Judson King (1971) states:

“Distillation is an energy-separating-agent equilibration process, and hence is desirable from an energy consumption viewpoint when staging is required. Distillation involves no solid phases, and hence enjoys an advantage relative to crystallization, which is another energy-separating-agent equilibration process. No contaminating mass-separating-agent is added in distillation, and it is easily staged within a single vessel. Because of this favorable combination of factors, it is no accident that distillation is the most frequently used separation process in practice, at least for large-scale operations. In fact, a sound approach to the selection of appropriate separation processes is to begin by asking ‘Why not distillation?’”

While continuous distillation dominates in large-scale operations, batch distillation has economical and operational advantages in many small-scale applications. Diwekar and Madhavan (1991c) state: “Batch distillation is preferable to continuous distillation where small quantities of high technology (and/or) high value-added chemicals and biochemicals are to be separated. The batch unit requires less capital for separating relatively pure components.” Luyben (1988) echoes: “Even though batch distillation typically consumes more energy than continuous distillation, it provides more flexibility and involves less capital investment. Since energy costs are not too significant in small-volume, high-

value products, batch distillation is often attractive for this class of products.” Al-Tuwaim and Luyben (1991) explain: “...a single column can handle any number of components. To achieve the same results using a continuous distillation system, NC-1 columns would typically be required for a system of NC components.” They continue: “Batch distillation columns play an important role in batch processes.” Galindez and Fredenslund (1988b) explain:

“Batch distillation may be preferable to continuous distillation where relatively small quantities of material are to be separated at irregularly scheduled periods. The most outstanding attribute of batch distillation is its flexibility. Little change is required when switching from one mixture to another. Reflux ratio and throughput can be varied easily. No balance of feed and drawoff need be maintained. In situations where the composition of the feed may change frequently or where different mixtures must be handled, the versatility of the batch distillation unit is excellent.”

One can envision a plant producing specialty chemicals where a few batch stills separate the products of many different batch reactors. Such a plant would enjoy these economical and operational advantages.

These advantages have placed batch distillation in many important applications. “Batch distillation is one of the most widely used separation processes in the manufacture of specialty chemicals. Specialty chemicals represent about 15% of worldwide chemicals production, with approximately \$150 billion produced annually” (Sundaram and Evans, 1993). Hard liquor is a commodity chemical produced by batch distillation. Recovery of acids in semiconductor processing is an example of batch distillation used for recycling wastes (Davison, 1992; SF Examiner, 1990).

1.2 Simulation of Batch Distillation

Batch distillation is an important process; however, it is not a simple one.

Luyben (1988) and Al-Tuwaim and Luyben (1991) state:

“The batch distillation process is characterized by unsteady-state conditions. This means that the compositions are functions of time. A large number of design and operating parameters must be optimized in order to design and operate the column: the number of trays, the size of the initial charge to the still pot, and the reflux ratio as a function of time (during product withdrawal periods and during the slop-cut periods).”

Because the process is so complex, optimal design and operation require analysis, not just experience. Sundaram and Evans (1993) state:

“In contrast to continuous distillation, until recently there have been few computer tools available for computer simulation and optimization of batch distillation. Batch distillations are performed based on trial and error experience, and the operation can be far from the economical optimum. There is a real need for systematic methodologies for the design and operation of batch separations.”

Process simulation entails three basic steps: 1) formulating a mathematical model of a physical process, 2) specifying process conditions as inputs to the model, and 3) solving the model to see how the process behaves. Using the Hagen-Poiseuille equation with a specified pressure drop to calculate flowrate through a pipe is a simple process simulation (Bird, et al., 1960). Writing a FORTRAN program, specifying feed and pressure, and calculating the products of an adiabatic flash is a more involved process simulation. Calculating the compositions and states of streams in a process plant using a general purpose flowsheet simulator is an example of large-scale process simulation.

Simulation is fundamental to engineering practice, because it predicts process behavior. The ASPEN PLUS Manual (1987) describes the benefits of process simulation:

“During process design, once the decision has been made to build a new plant or to modernize an existing plant, ASPEN PLUS models may be used to study trade-offs, to investigate off-design operation, and to investigate the flexibility of the plant to handle a range of feedstocks. Simulation studies during process design can avoid costly mistakes before committing to plant hardware. Process engineers can use a simulation model to optimize the design of their process by making a series of case studies to ensure that the plant will work properly under a wide range of operating conditions.

For an existing plant, an ASPEN PLUS model can serve as a powerful tool for plant engineers to improve plant operations, to improve yield and throughput, and to reduce energy use. The model can be used to determine changes in operating conditions needed to accommodate changes in feedstocks, changes in product requirements, and changes in environmental conditions. The model can guide plant operations to reduce costs and improve productivity. Finally, the modeling can be used to study possible plant modifications for ‘debottlenecking’ or for revamping the plant to incorporate technology advances such as an improved catalyst, a new solvent to a new process unit.”

Both process simulation and pilot-scale experiments can supply the information necessary for process design or optimization. Experiments are frequently expensive, time-consuming, and are often impossible in operating plants. Process simulation is indispensable to engineering practice, for situations where experiment is impracticable.

1.2.1 Batch Distillation Simulation with Rigorous Fully Dynamic (RFD) Models

Current batch distillation simulations use the rigorous, fully dynamic or quasi-steady-state column approximation methods. The RFD approach entails deriving the set of differential and algebraic equations that describe the process

and solving the system numerically. This set of equations includes: 1) material and energy balances, 2) vapor-liquid equilibria, 3) mass and heat transfer relations and 4) fluid dynamics equations. This approach has been successful for batch distillation simulation in numerous applications (see Chapter 2).

RFD is a successful, but complex technique for batch distillation simulation. According to Seider (1984):

“(The programs) require lengthy operation of large computers . . . The equations may be difficult to integrate rapidly and accurately because they may constitute a so-called stiff system as considered by Gear (1971). When such systems are integrated by simple explicit methods, the time step cannot be too large or small, or the solution will suffer from instability or truncation-error.”

The fully dynamic approach buys rigor for speed, which is a reasonable exchange, especially when closely analyzing one column under one set of conditions. Engineers often need to solve their models tens or hundreds of times when optimizing column design or operating conditions or when evaluating a control strategy, and then the calculation time takes its toll.

Diwekar (1991a) states: “Another major issue in batch process design or synthesis is operational flexibility, which gives rise to a large number of alternative evaluations. Use of rigorous models becomes prohibitively expensive because of large computational efforts involved and extensive data and memory requirements.” This burden drives some to forsake the rigorous model approach for faster methods such as the quasi-steady-state column approximation approach.

1.2.2 Quasi-Steady-State Column Approximation (QSSCA) Models

The QSSCA approach speeds calculations by exploiting the stiffness of the system. L.M. Rose (1985) explains:

“... the system of differential equations (has) two regions for the time constants. The hold-up equations (describing column trays) have time constants in seconds and the (equations describing) boiler contents (have time constants) in hours. An established technique for treating systems with two ranges of time constants is to assume that the set with the small time constant so quickly approaches equilibrium that during a large time step appropriate for the large time constant system, the variables associated with the smaller time constant remains constant. Hence, . . . the column calculation reverts to the same set of equations as for continuous distillation.”

This approach inherently can run much faster than an RFD simulation because it eliminates most of the differential equations, and the ones that remain have longer time constants, appropriate for the boiler. In addition, the QSSCA approach can take advantage of specialized programs for solving continuous distillation problems. These programs are much faster and more stable than the general programs for solving systems of ordinary differential equations used in the RFD approach.

The QSSCA approach has simulated batch distillation in many applications (see Chapter 2). Though fast and popular, the steady column approach has drawbacks, because it forgoes dynamic description of the column and therefore relinquishes information on the time to start-up or respond to changes. Holdup has some effects on separation and thus can affect accuracy of simulation, in some cases. These are reasons to do preliminary work with the speed of the steady approach and finally check the simulation with the accuracy of the fully

dynamic approach.

Despite its advantages and successes, batch distillation simulation using the QSSCA approach is not easily available to working chemical engineers who use common flowsheet simulators. The major American process simulation packages use RFD-based simulations, such as BATCHFRAC in ASPEN PLUS (Boston et al., 1981). A comprehensive literature search found that simulation using the QSSCA is in only one flowsheet simulator, SIMBAD, by academics in Argentina (Chiotti and Scenna, 1989). Publications on the QSSCA-based simulations describe its results in detail, but they are sketchy about the procedures. The papers review the principles, but this generally is not sufficient to instruct a chemical engineer on construction of his or her own simulation program. Thus, there is an unmet need for an easy procedure for implementing batch distillation simulation using the QSSCA in a widely available flowsheet simulator.

1.3 Research Objective and Hypotheses

This research has an objective to develop and investigate a straight-forward implementation of the quasi-steady-state column approximation approach to batch distillation simulation on a commercial modular process simulator.

To achieve this objective, the following hypotheses are evaluated:

- 1) A batch distillation simulation based on the QSSCA approach can be implemented on a prototypical, commercial, modular process simulator.
- 2) Results from this simulator are comparable with the results of published simulations using the QSSCA approach.

3) A general paradigm can be illustrated to facilitate implementation of this simulation technique.

Terms in the hypotheses are defined as follows:

Batch distillation simulation based on the QSSCA approach is the prediction of distillate or tops and raffinate or bottoms composition and volume during the process.

The *quasi-steady-state column approximation* states that transitory behavior of the column is so brief that it can be neglected relative to longer transients in the boiler, because material holdup in the rectification column is negligible compared with the holdup in the boiler.

Implementation means developing the model using the primary commands available in the simulation language without writing specific modules in a lower-level programming language, such as FORTRAN.

ASPEN PLUS is a *prototypical, commercial flowsheet simulator*, because it is one of the major, commercial simulators widely available in the United States.

Comparison with other results is comparison of the course of distillate and boiler composition and volume predicted by this simulation with published values from experiments and other simulations.

1.4 Additional Advantages of this Effort

Besides meeting these needs, other advantages accrue from integrating batch distillation simulation using the QSSCA approach into a general-purpose process simulator (GPPS). Integration transparently incorporates batch distilla-

tion results into simulation of a complete process. It gives the batch distillation simulator access to the continuous distillation routines and physical property models and databases in the GPPS. These modules are some of the best available, and they are continuously maintained and improved by the GPPS vendor. Availability of batch distillation simulation by both QSSCA and RFD approaches on one GPPS allows quick calculations by QSSCA to optimize preliminary design, and more rigorous calculations by RFD to check final design.

Besides creating a design tool, this investigation suggests the parameters that are important in the implementation of the approach and their effects on the calculations. Significant parameters may include: 1) step-size for integrating composition change in the boiler, 2) model for the steady-state distillation column, and 3) details of programming on the process simulator. The implementation procedure and the identification of important parameters are generally applicable principles that apply to other GPPS's besides ASPEN PLUS.

This approach probably is widely applicable, but it surely is not universal. Therefore, in each new application, the user must independently assess the accuracy of its predictions before using it for design.

CHAPTER 2. LITERATURE REVIEW

This review traces the history of batch distillation simulation, based on a general literature search and specific reviews by Seader (1984), Diwekar and Madhavan (1991c), Sundaram and Evans (1993) and others. It also compares the primary, current simulation techniques: the fully dynamic and quasi-steady-state approaches.

2.1 Rayleigh Equation for a Simple Batch Still

Mathematical modeling of batch distillation began with the analysis of a simple batch still: a boiler directly connected to a condenser. The first publication was Lord Rayleigh's 1902 paper "On the Distillation of Binary Mixtures." "Young (1922), Rosanoff (and coworkers) (1914), Lewis (1909), Lewis and Robinson (1922), and Peters (1923) all discussed the theory of...simple distillation," according to Rose and Welshans (1940a).

Lord Rayleigh's analysis applies to multicomponent as well as binary mixtures. This simple yet rigorous treatment begins with overall and component material balances on the boiling liquid. In the following equations, V and L are the mols of vapor and liquid, and x and y are the instantaneous vapor and liquid mol fractions, respectively. The overall balance states: the increment of vapor (dV) equals the decrement of remaining liquid in the still (dL).

$$dV = -dL$$

The component balance states: the increase of a component in the vapor ($y dV$) equals the decrease of that component in the liquid ($d(Lx)$). This equals the component's mole fraction times the moles of liquid decrement ($x dL$) added to the decrease in the component's mole fraction multiplied by the moles of liquid remaining ($L dx$).

$$y dV = -d(Lx) = -(x dL + L dx)$$

Combining and rearranging these differential balances to eliminate dV yields:

$$-y dL = -(x dL + L dx)$$

$$(x - y) dL = -L dx$$

$$\frac{-dL}{L} = \frac{dx}{(x - y)}$$

$$\int_{L_0}^L \frac{-dL}{L} = \ln\left(\frac{L_0}{L}\right) = \int_{x_0}^x \frac{dx}{(x - y)}$$

The last equation can be integrated from the beginning of distillation at time zero, when L is L_0 , x is x_0 and y is y_0 , to some later time. Integration of the left-hand-side results in a logarithmic relationship, $\ln(L_0/L)$. The right-hand-side, $\int dx/(x-y)$, can be integrated with a vapor-liquid equilibrium function, assuming well-mixed vapor and liquid phases and specified pressure. Integration always can be performed numerically or graphically. For mixtures with constant relative volatility's, simplified analytical expressions can be found for the integrals (Seader, 1988). This integral equation relates liquid and vapor compositions to liquid boil-up.

The integrated energy balance relates boil-up to the known heat rate to the still. Integrating liquid boil-up with the equilibrium vapor composition finds the accumulated distillate composition.

2.2 Early Models of Batch Rectification

The simple batch still has limited utility because it consists only one separation stage. Finer separation requires a rectifying column that includes numerous stages on top of the boiler. Mathematical modeling of batch rectification began in the late 1930's and 1940's, when investigators developed design methods for stills operating with either 1) substantially total reflux, 2) varying reflux and constant distillate composition, or 3) constant reflux and varying distillate composition. By 1940, Rose derived "a general expression for the calculation of such batch distillation curves (composition of distillate cuts plotted against percentage of charge distilled), and the calculations for certain limiting cases of distillation under substantially total reflux," according to Smoker and Rose (1940). In 1940, Rose and Welshans used Fenske's total reflux equation to find the relationship between boiler and distillate composition and investigated the effects of relative volatility and number of plates on the sharpness of separation. In 1937, Bogart developed a design method for a batch rectification producing constant overhead composition by increasing the reflux ratio. Figure 2-1 illustrates this operation on a McCabe-Thiele (1925) x-y diagram with an equilibrium curve, a 45-degree or total reflux line and several operating lines (Seader, 1984).

Figure 2-1. McCabe-Thiele Diagrams for Batch Distillation

Perry's Handbook (1984) describes the basis of the McCabe-Thiele diagram. The operating line slope is the ratio of liquid to vapor flows. This slope increases during distillation and generates a family of operating lines. The operating lines all intersect the 45-degree line at the constant overhead composition. From this intersection, the column's theoretical plates are stepped-off between the operating line and the equilibrium curve to find the boiler composition. In 1940, Smoker and Rose modeled batch rectification with (finite) constant reflux ratio, and therefore changing distillate composition. Their method uses a McCabe Thiele diagram to find the relationship between boiler and distillate composition for integration of the Rayleigh equation. Their x-y diagram, Figure 2-1, also has an equilibrium curve, a 45-degree line and several operating lines (Seader, 1984). The operating line slope is the constant liquid-to-vapor flow ratio. The intersection of the operating and 45-degree lines is the distillate composition, which becomes increasingly concentrated with the less volatile component as distillation proceeds, generating a family of operating lines. From the distillate intersection, the column's theoretical plates are stepped-off between the operating line and the equilibrium curve to find the boiler composition.

2.3 Investigations of Hold-up Effects

McCabe-Thiele graphical methods are only exact for an ideal binary system with equimolar overflow in an adiabatic column with negligible holdup and uniform pressure. Column holdup is the inventory of liquid and vapor in the trays

or packing and condenser. In 1940, Rose and Welshans extended their model of batch distillation with substantially total reflux to include holdup. They found "that the size of the intermediate (slop) cut for maximum sharpness of separation (of a binary mixture) varies in an approximately linear fashion (increasing) with the holdup..." In 1941, Colburn and Stearns developed a theoretical and experimental basis for explaining the first two effects of holdup: provision of capacity or "inertia" in the column and depletion of lighter components from the charge in the boiler (Seader, 1988). "As both these effects occur at the same time and change in importance during the course of distillation, it is difficult, without rigorous calculations, to predict whether the overall effect of hold-up will be favorable or detrimental; it is equally difficult to estimate the magnitude of the holdup effect," according to Seader (1984).

This uncertainty, and the uncertainty encountered in applying McCabe-Thiele graphical methods approximately to systems violating their assumptions, encouraged over-design of batch distillation columns, that is, using too many stages or too much reflux. Elimination of these uncertainties motivated development of rigorous batch distillation models. Between 1950 and 1953, Rose, Johnson and Williams studied holdup effects experimentally and theoretically. They developed differential material balances, and solved them by plate-to-plate calculations, either by hand or on early IBM computers. In 1951, Pigford, Tepe and Garrahan predicted the effects of holdup by modeling a batch still with seven

theoretical stages on a mechanical analog computer. They found “a general tendency for the size of the intermediate fraction (slop cut) to increase with increasing holdup,...(except) in the case of certain easy separations...(where) the size of the intermediate cut decreases at first and then increases with increasing holdup.”

2.4 Dynamic Column Models including Energy and Material Balance

Rigorous mathematical models of batch distillation involve differential equations for overall and component material balance and energy balance in the boiler, column and condenser. In 1960, Huckaba and Danly simulated binary batch distillation with a computer program, performing mass and energy balances on trays with constant mass holdup, and validated their simulation with experimental data. In 1963, Meadows modeled multicomponent batch distillation, including mass, energy and volume balances on trays with constant volume holdup. In 1967, Barb and Holland modeled all phases of batch column operation, including startup and different product periods. Distefano extended Meadows' model in 1968, and successfully simulated several commercial batch distillation columns. “The Distefano model is the most cited rigorous model for batch distillation and most of the studies and simulation models that have appeared since 1968, e.g., Boston et al. (1981), are based on this model,” according to Diwekar (1991a).

Batch distillation models are available in several commercial, general-pur-

pose process simulators. CHEMCAD by Chemstations has "BATCH" for batch distillation simulation. PRO/II by Simulation Sciences has "BATCHEM" which uses Distefano's model. ASPEN PLUS by Aspen Technology has "BATCHEM" which also uses Distefano's model. BATCHEM incorporates the specification flexibility found in continuous column simulators, according to Seader (1984):

"(BATCHEM) divides the batch distillation process into a sequence of operation steps. At the beginning of each step, the reboiler may receive an additional charge, distillate or sidestream receivers may be dumped, and a feed reservoir may be refilled. Specifications for an operation step include feed, sidestream withdrawal, and tray heat-transfer rates. In addition any two of the following five variables must be specified: reflux ratio, distillate rate, boil-up rate, condenser duty, and reboiler duty. Finally, column configuration and operating conditions (number of stages, holdups, tray pressures,...) can be changed at the beginning of each operation step. An operation step is terminated when a specified criterion, selected from the following list, is reached: a time duration; a component purity in the reboiler, distillate, or distillate accumulator; an amount of material in the reboiler or distillate accumulator; or a reboiler or condenser temperature."

In recent publications, researchers reported modeling batch distillation together with chemical reaction, packed columns and optimization of operating strategy. Ruby (1978), Egly (1979) and their coworkers, and Cuille and Reklaitis (1986) extended Meadows' model to account for liquid-phase chemical reactions. Reuter and colleagues (1989) used their approach to simulate esterification in a batch reaction driven to completion by distillation. In all the studies noted above, researchers derived their models for batch distillation in plate columns. Aly (1987, 1990a,b), Jahromi (1982), Domenech and their coworkers derived models

for packed columns and found that axial dispersion is significant, but radial dispersion is negligible. In the late 1980's and the 1990's, some researchers saw their batch distillation models not as ends in themselves, but as tools for investigating the optimization of batch still design and operation. Luyben (1988) and Farhat and coworkers (1990) studied the effect of fixed and variable reflux ratio on the quantity of product produced, and Quintero-Marmol and Luyben (1990) and Mujtaba and Macchietto (1988) investigated slop-cut recycling strategies and found approaches that are significant improvements over simply adding the slop cut to the next batch. Diwekar and Madhavan (1991a,b,c) developed a short-cut method for preliminary design and analysis of batch columns. Diwekar and her associates (1987, 1989, 1992) used this method to solve optimal design, operation and control problems.

The algebraic and ordinary differential equations in a rigorous batch distillation model constitute an initial value problem. It is generally impossible to solve these models analytically, because the equation set is very large, and the thermodynamic functions generally are nonlinear. Since the application of large digital computers to chemical engineering in the 1960s, numerical solutions have been developed; Meadows (1963) used finite differences, and Distefano (1968a,b) compared 11 methods. Their programs required "lengthy operation of large computers," because "the equations may be difficult to integrate rapidly and accurately because they may constitute a so-called stiff system as considered by

Gear (1971),” according to Seader (1984). Boston (1978) invented an “inside-out” algorithm, “...a robust and efficient method which could cope with the stiff nonlinear equations produced by the integration formula,” according to Sundaram and Evans (1993). Others turned to stable implicit methods; for example, Gallun and Holland (1982) used an improved Gear method, Holland and Liapis (1983) and Reuter and coworkers (1989) used two-point implicit methods, Aly and colleagues (1987, 1990a,b) used a Galerkin-type finite element method, and Hitch and Rousseau (1988) used a relaxation method, which they described as slow but stable. Seeming to ignore the stiffness problem, Al-Tuwaim (1991), Luyben (1988, 1990) and Quintero-Marmol (1990, 1992) worked together and used a modified Euler method, but they frequently neglected energy balances and avoided nonlinear thermodynamics.

2.5 Quasi Steady-State Column Models

The fully dynamic approach obtains stability and rigor at the cost of speed. This is a reasonable exchange, especially when closely analyzing one column under one set of conditions. However, an engineer may solve a model tens or hundreds of times when optimizing column design or evaluating an operating strategy, and then the calculation time takes its toll. This burden drove Diwekar to replace the rigorous model approach with short-cut methods that approximate the column as a whole. Luyben grossly simplified his model to speed calculations, and others took the quasi-steady-state column approximation (QSSCA)

approach.

The QSSCA approach speeds calculations by exploiting the stiffness of the system. Rose (1985) explains it, with reference to the relaxation method, but his discussion is generally applicable:

“(The) relaxation method is not a very quick way of achieving convergence in (a system of equations describing) a column, and this problem is magnified when it is coupled with the boiler mass balance equations. The resulting system is a system of differential equations with two regions for the time constants. The hold-up equations (describing column trays) have time constants in seconds and the (equations describing) boiler contents (have time constants) in hours. It is well known that such equations are difficult to integrate numerically (they are stiff), and the (time) step length must be very small and computer times correspondingly large.

The situation is intensified when packing is used for the column internals, because here the holdup is a thin film on the packing, and the boiler may contain 10 tons of liquid! The less important the holdup ... the more difficult ... the calculation to predict its effect, because the system of differential equations becomes stiffer!

Unfortunately, this approach does not help to solve our batch design problem of choosing a degree of detail commensurate with the equipment costs. Our systems of equations can be solved, but computer time hundreds of times longer than the time for steady state distillation is obtained, and design costs are inappropriate to the size of equipment being designed.

An established technique for treating systems with two ranges of time constants is to assume that the set with the small time constant so quickly approaches equilibrium that during a large time step appropriate for the large time constant system, the variables associated with the smaller time constant remain constant. Hence, Equation 5.12 (the component material balances on column trays) has a zero right-hand-side (accumulation terms), and the column calculation reverts to the same set of equations as for continuous distillation.”

In several recent publications, researchers have used the QSSCA approach to simulate batch distillation. Rose (1979, 1985) used it as the basis of

his simulator BATCH. According to Logsdon et al. (1990), "The no-holdup simulation model has been used by Diwekar et al. (1989) and Domenech and Enjalbert (1981) for screening purposes in preliminary design." Bernot and colleagues (1990, 1991) used QSSCA to investigate azeotropic batch distillation, and Farhat and collaborators (1990) used it to study optimization of multifraction batch distillation. Quintero-Marmol and Luyben (1990, 1992) compared simulations by RFD and QSSCA, and found the results similar. Nad and Spiegel (1987) compared the QSSCA and RFD approaches, and found QSSCA 20 times faster, according to Galindez and Fredenslund (1988b). Galindez and Fredenslund combined QSSCA with an existing continuous column simulator to take advantages of the highly developed algorithms (UNIDIST and UNIFAC) in it. Chiotti and Scenna (1989) incorporated QSSCA batch distillation simulation into SIMBAD, his general purposes modular process simulator.

Though fast and popular, QSSCA has drawbacks. It absolutely drops dynamic description of the column, and thus relinquishes information on the time to reach steady state or respond to changes. Holdup has some effects on separation, and in some cases this can affect the accuracy of simulation. These are reasons to do preliminary work with the speed of QSSCA and finally check it with the accuracy of the fully dynamic approach.

CHAPTER 3. METHODS DEVELOPMENT

3.1 Simulating Batch Processes with Steady-State Models

Batch process simulators that use a series of continuous process models rely on the following premise: at any instant, a batch process with material in the batch tank produces the same product as the same process running continuously with the same material as feed. Diwekar and Madhavan (1991c) state the premise as follows: "This (short-cut) method is based on the reasonable approximation that the batch distillation column can be considered as a continuous distillation column with changing feed. In other words, the bottom product of one time step forms the feed of the next time step." This premise is a basis for this modeling effort, and it is substantiated based on material and energy balances and equilibrium thermodynamics.

In the premise, the phrase "at any instant" means during an interval of time so short that the amount of product withdrawn from the batch process is small compared to the size of the batch tank. Alternatively, a small product increment could replace the short time interval. The phrases "a batch process" and "the same process running continuously" mean that the batch and continuous processes have the same process flow diagram, equipment design, heat input, etc. The phrases "material in the batch tank" and "the same material as feed" mean that the feed composition, state and quantity per unit time in the model con-

tinuous process equals the composition, state and quantity of material in the batch process over the time interval being simulated. The phrase "produces the same product" means that the quantity, composition and state of product are the same in both processes, and this is the claim of the premise.

Material balance sets a necessary condition for equality of products from batch and steady processes: over the differential time interval being modeled, the feed to the steady process must equal the quantity and composition of the initial inventory in the batch process. This is demonstrated by the following overall and component material balance equations (input = output + accumulation). They specifically apply to binary distillation, operating steady-state and batch-wise in the single-stage columns shown in Figure 3-0. Similar balances can be written for multicomponent distillation in multistage columns. Their symbols are defined in Figure 3-0 and below.

Steady State

Batch

Reboiler

$$F + L_1 = B + V_0 + 0$$

$$0 + L_1 = B + V_0 + \frac{dA_0}{dt}$$

$$Fz + L_1x_1 = Bx_0 + V_0y_0 + 0$$

$$0 + L_1x_1 = Bx_0 + V_0y_0 + \frac{dA_0x_0}{dt}$$

Figure 3-0. Generalized Stills for Material and Energy Balances

Batch

Steady State

Steady StateBatchColumn Stage

$$V_0 + L_n = V_1 + L_1 + 0$$

$$V_0 + L_n = V_1 + L_1 + \frac{dA_1}{dt}$$

$$V_0 y_0 + L_n x_n = V_1 y_1 + L_1 x_1 + 0 \quad V_0 y_0 + L_n x_n = V_1 y_1 + L_1 x_1 + \frac{dA_1 x_1}{dt}$$

Condenser

$$V_1 = D + L_n + 0$$

$$V_1 = D + L_n + \frac{dA_n}{dt}$$

$$V_1 y_1 = D x_n + L_n x_n + 0$$

$$V_1 y_1 = D x_n + L_n x_n + \frac{dA_n x_n}{dt}$$

Adding the balances gives:

$$F = B + D$$

$$0 = B + D + \frac{dA_0}{dt} + \frac{dA_1}{dt} + \frac{dA_n}{dt}$$

$$F z = B x_0 + D x_n$$

$$0 = B x_0 + D x_n + \frac{dA_0 x_0}{dt} + \frac{dA_1 x_1}{dt} + \frac{dA_n x_n}{dt}$$

Applying the QSSCA, which says that dA_0/dt is much larger than $(dA_1/dt + dA_n/dt)$ because A_0 is much larger than $(A_1 + A_n)$, and rearranging, gives:

$$F = B + D$$

$$-\frac{dA_0}{dt} = B + D$$

$$F z = B x_0 + D x_n$$

$$-\frac{dA_0 x_0}{dt} = B x_0 + D x_n$$

Concluding: If steady state $F = -\frac{dA_0}{dt}$ batch,

then, steady state $(B + D) = (B + D)$ batch.

Likewise: If steady state $Fz = -\frac{dA_0x_0}{dt}$ batch,

then, steady state $(Bx_0 + Dx_n) = (Bx_0 + Dx_n)$ batch.

where, F, D, B, L, V Feed, Distillate, Bottoms, Liquid, Vapor flowrates

A Vapor and Liquid Accumulation

z, y, x Mol fractions of a component in F, V or D, L or B

0, 1, n Subscripts denoting Reboiler, Column, Condenser

The feed to the steady process must equal the whole charge to the batch process, not just the quantity distilled, because the program empties the batch still after each step and uses the bottoms as the charge for the next step. These are necessary, though not sufficient, conditions for process equivalence.

The material balances above and the energy balance below apply exactly to differential time intervals and differential fluid elements. The quasi-steady-state column approximation says that they also apply approximately to short time steps. It says that, over a small change in batch still concentrations, the material and energy streams of the batch system are approximated by those of a continuous system. In other words, batch distillation is a quasi-static process. The stage-wise equilibrium approximation says that the balances also apply to all the material on a separation stage. That is, the vapor and liquid phases on each stage are well-mixed and equilibrated at any instant. In other words, the re-

sponse to perturbations away from well-mixed equilibrium is rapid relative to other time lags in the system. This approximation is used to calculate concentrations and other state variables without involving irreversible thermodynamics and transport phenomena. It is common in both batch and continuous process modeling, and it is corrected on the flowsheet simulator by using a stage efficiency parameter.

Energy balance sets another necessary condition for products of batch and steady processes to be equal: the sum of feed enthalpy and heat into the steady process must equal the sum of inventory enthalpy and heat into the batch process over the differential of time being modeled. Two processes meet this condition if the composition, state and temperature of feed to the continuous process equal the composition, state and temperature of inventory in the batch process, and the heat into the two processes is equal. The following energy balance equations demonstrate this. Again, they apply to the steady and batch distillation columns in Figure 3-0.

Steady State

Batch

Reboiler

$$FH_F + L_1H_{L1} + Q_0 = BH_{L0} + V_0H_{V0} + 0$$

$$Q_0 + L_1H_{L1} = BH_{L0} + V_0H_{V0} + \frac{dA_0H_{M0}}{dt}$$

Steady State

Batch

Column Stage

$$V_0 H_{V0} + L_n H_{Ln} = L_1 H_{L1} + V_1 H_{V1} + 0$$

$$V_0 H_{V0} + L_n H_{Ln} = L_1 H_{L1} + V_1 H_{V1} + \frac{dA_1 H_{M1}}{dt}$$

Condenser

$$V_1 H_{V1} + Q_n = L_n H_{Ln} + DH_{Ln} + 0$$

$$V_1 H_{V1} + Q_n = L_n H_{Ln} + DH_{Ln} + \frac{dA_1 H_{Mn}}{dt}$$

Adding the balances gives:

$$FH_F + Q_0 + Q_n = BH_{L0} + DH_{Ln}$$

$$Q_0 + Q_n = BH_{L0} + DH_{Ln} + \frac{dA_0 H_{M0}}{dt} + \frac{dA_1 H_{M1}}{dt} + \frac{dA_1 H_{Mn}}{dt}$$

Applying the QSSCA, which says that $dA_0 H_{M0}/dt$ is much larger than $(dA_1 H_{M1}/dt + dA_n H_{Mn}/dt)$ because A_0 is much larger than $(A_1 + A_n)$, and rearranging, gives:

$$FH_F + Q_0 + Q_n = BH_{L0} + DH_{Ln}$$

$$-\frac{dA_0 H_{M0}}{dt} + Q_0 + Q_n = BH_{L0} + DH_{Ln}$$

Concluding: If steady state $(FH_F + Q_0 + Q_n) = (-\frac{dA_0 H_{M0}}{dt} + Q_0 + Q_n)$ batch,

then, steady state $(BH_{L0} + DH_{Ln}) = (BH_{L0} + DH_{Ln})$ batch.

where, H Molar enthalpy (a state function of composition, temperature, pressure.)

F, L, V, M Subscripts denoting Feed, Liquid, Vapor, Mixed

Meeting the energy balance condition ensures top and bottom products having the same state and temperature in the two processes, given that they have the same flowrates and compositions for material balance reasons.

Material and energy balances involve the extensive properties of materials in processes, and they set some of the conditions for process equivalence. Equilibrium thermodynamics sets other, complementary conditions on the intensive properties. The same equations determine equilibrium in steady and batch processes.

Steady State

Batch

Reboiler

$$y_0/x_0 = K_0 = K(T_0, P_0, x_0)$$

$$y_0/x_0 = K_0 = K(T_0, P_0, x_0)$$

$$H_{L0} = H_{L0}(T_0, P_0, x_0)$$

$$H_{L0} = H_{L0}(T_0, P_0, x_0)$$

$$H_{V0} = H_{L0}(T_0, P_0, y_0)$$

$$H_{V0} = H_{L0}(T_0, P_0, y_0)$$

$$H_{M0} = (A_{L0}H_{L0} + A_{V0}H_{V0})/(A_{L0} + A_{V0})$$

$$H_{M0} = (A_{L0}H_{L0} + A_{V0}H_{V0})/(A_{L0} + A_{V0})$$

Steady StateBatchColumn Stage

$$y_1/x_1 = K_1 = K(T_1, P_1, x_1)$$

$$y_1/x_1 = K_1 = K(T_1, P_1, x_1)$$

$$H_{L1} = H_{L1}(T_1, P_1, x_1)$$

$$H_{L1} = H_{L1}(T_1, P_1, x_1)$$

$$H_{V1} = H_{L1}(T_1, P_1, y_1)$$

$$H_{V1} = H_{L1}(T_1, P_1, y_1)$$

$$H_{M1} = (A_{L1}H_{L1} + A_{V1}H_{V1})/(A_{L1} + A_{V1})$$

$$H_{M1} = (A_{L1}H_{L1} + A_{V1}H_{V1})/(A_{L1} + A_{V1})$$

Condenser

$$y_n/x_n = K_n = K(T_n, P_n, x_n)$$

$$y_n/x_n = K_n = K(T_n, P_n, x_n)$$

$$H_{Ln} = H_{Ln}(T_n, P_n, x_n)$$

$$H_{Ln} = H_{Ln}(T_n, P_n, x_n)$$

$$H_{Vn} = H_{Ln}(T_n, P_n, y_n)$$

$$H_{Vn} = H_{Ln}(T_n, P_n, y_n)$$

$$H_{Mn} = (A_{Ln}H_{Ln} + A_{Vn}H_{Vn})/(A_{Ln} + A_{Vn})$$

$$H_{Mn} = (A_{Ln}H_{Ln} + A_{Vn}H_{Vn})/(A_{Ln} + A_{Vn})$$

where, K Vapor/Liquid Equilibrium Constant

T Temperature

P Pressure

The equilibrium conditions are the same in the steady and batch processes; the following thought experiment elucidates this.

Two identical portions of material, Fz are fed to a steady process and made the inventory of a batch process. The two mechanically identical processes are a binary vapor/liquid equilibrium, so Phases=2 and Components=2. Gibbs' Phase Rule states that Degrees of Freedom = 2 - Phases + Com-

ponents. If two state variables, say temperature and pressure, are specified the same in both cases, the two remaining degrees of freedom are taken and the two systems are completely determined. Then before product removal, the same material is under the same thermodynamic conditions in the two systems, so both systems come to the same equilibrium.

This result really is not surprising. There is no difference, thermodynamically, between a continuous process where F mol/min of feed of some composition are heated at Q Joules/min at pressure P atm and products D and B are discharged to holding tanks, and a batch process where F mols of feed of the same composition are heated with Q Joules at pressure P atm for one minute and products D and B are unloaded from the batch tank. The same starting material receives the same energy under the same conditions of thermodynamic state variables, therefore the products are the same, if both processes reach equilibrium and the phases separate well. The difference between the continuous and batch processes is their path, not their endpoints, and only endpoints matter in equilibrium. Thus, equilibrium thermodynamics sets another necessary condition for process equivalence: a number of state variables, equal in number to the degrees of freedom, must be set the same in both the batch and steady process.

Figure 3-1 illustrates these principles on McCabe-Thiele diagrams for a batch distillation and a continuous distillation simulating it. The batch tank and the continuous feed have the same composition and quantity of material, so the operating line endpoint is the same on both diagrams. Since the heat

Figure 3-1. McCabe-Thiele Diagrams for Distillation Simulation

Batch

Steady State

rates and equipment design are the same, the vapor/liquid ratio is the same in both columns and the operating line has the same slope on both diagrams. With the same end point and slope, the operating line is the same on both diagrams. Since the processes are the same, both diagrams only have an operating line for rectification. The columns operate at the same thermodynamic state on the same material, so the equilibrium curve is the same. The $x=y$ line is the same on both diagrams, and it represents the streams crossing in the total condenser on top of both columns. Thus, all of the guide lines are the same on both diagrams. When the same number of stages are stepped off on both diagrams, they predict the same distillate, confirming the simulation. The diagrams in Figure 3-1 represent one step-of-integration in the simulation of the process. As the distillation proceeds the boiler composition changes and new operating lines represent the process, as shown on Figure 2-1. Each operating line is another step in the integration of the process. The more rapidly the operating line changes, the finer the steps-of-integration.

3.2 Implementing this Batch Simulation Approach in a GPPS

Having established that a steady process model can simulate a step in a batch process, the next step is to use this premise in a computer program to simulate batch distillation. This program must perform two interacting tasks: 1) column simulation to find product composition from boiler composition, that is, $y = y(x)$, and 2) integration or differential equation solution to relate final distillate

product to the initial still charge, that is, $\int d(Lx) = \int d(Vy)$. This section describes the programming for column simulation from the top-down: the programming environment, the thermodynamics model, the column simulator, and the simulation of column holdup. To help concretize this general discussion of principles, Exhibits 4-1, 4-2, 4-3 and Appendix A show example programs. The programs' specifics apply to test cases described in the next chapter.

Galindez and Fredenslund (1988b) and Chiotti and Scenna (1989) used preprogrammed subroutines for solving steady-state columns in their batch distillation simulations. Writing original software to model continuous rectification really is not necessary as a number of proven software packages are available. Among the best steady column simulators available are those in general-purpose process simulators such as ASPEN PLUS, Process, ChemCad, etc. Since they all have fine rigorous distillation models, the programmer can choose among them on peripheral considerations: cost, ease of use, etc. On these bases, ASPEN PLUS was chosen for this study.

Working within the general-purpose flowsheet simulator, the programmer must choose a model for thermodynamics-physical properties. It should represent the chemical system without using excessive computer time, considering the other approximations in the model. Since a goal of this work is to compare results this QSSCA model of batch distillation to similar simulations in the literature, UNIFAC/Redlich-Kwong, a properties model closely matching those used in the

published work, was chosen.

There are three choices for the distillation column model: 1) a column built of primitive unit operations like flashes, reactors and heat exchangers, 2) a rigorous, stage-by-stage column solver, or 3) a short-cut column solver. The sequence-of-flashes approach was tried and abandoned, because convergence would have required extensive FORTRAN programming, contrary the hypothesis of implementation using the primary commands available in the simulation language.

Distillation column solvers are specialists at solving convergence problems. Two basic types of analysis are available in distillation column solvers, rigorous or short-cut. Obviously, rigorous stage-by-stage calculations are more accurate than short-cut calculations that treat the column as a single entity. Rigorous solvers usually also accommodate a wider range of more detailed design specifications than short-cut solvers. However, short-cut solvers involve far fewer calculations and hence are much faster than rigorous solvers. The choice between rigorous and short-cut solvers is a choice between accuracy and speed. The recommended compromise is an extension of the advice for using RFD and QSSCA. Use QSSCA with short-cut models for preliminary design scouting, then use QSSCA with rigorous columns to optimize, and finally use RFD simulation to check the final design. In this study, programs were written with both rigorous and short-cut solvers.

If material and thermal holdups in the column are negligible, the specifications and conditions of steady and batch columns are the same, but if there are holdups, the specifications and conditions are inherently different. In continuous distillation, the material holdups on the trays and in the boiler and condenser are established during startup, and they are not taken from the feed during operation. Continuous process models, which only simulate operation after startup, can ignore material and thermal holdup. In batch processes, the batch charge must produce "products" in addition to the distillate and raffinate: the holdups. As the batch distillation proceeds, the holdups combine their material with the vapor and liquid rising and falling onto a stage, and as their compositions change, they act as sources and sinks of material; something that does not happen in steady-state processing. While steady and batch distillation are inherently different when there are holdups, the view of holdups as feed and product from each stage is the basis of a conception of a continuous column that can model to a batch column.

To model material and associated thermal holdups in batch distillation, the model must account for two considerations: carrying holdups from step-to-step and starting up the column. Galindez and Fredenslund's work (1988b) provides a way to simulate holdups by treating them as stage products from the previous step-of-integration that feed the next step-of-integration. They represent a tray's holdup as a stage product, a sidestream from the column tray, which comes from

stage j of the column at step $k-1$ of the integration, to stage j of the column at step k of the integration, and passes onto stage j of the column at step $k+1$ of the integration. Figure 3-2 compares their model which accounts for holdup in the column, with a simpler model that neglects holdup. The holdups pass from one integration step to the next, and thus stay in the column. Their quantities are constant until the end of the process, but their composition changes to reflect the changing composition on the trays.

To simulate the startup of such a column and establish the holdups, the model initially runs with total reflux, just as in real life. The program specifications divide the feed charge among the boiler and the holdups on the trays, all at the initial charge composition. The column then runs with total internal reflux. Each stage produces a product equal in quantity to its holdup feed, but with its composition reflecting the separation occurring in the column. This composition is fed to the corresponding tray in the column in the next step-of-integration, also operating with total internal reflux. Total reflux continues until the composition of holdups stabilizes, and then distillate production begins while holdup input and output continues. Figure 3-3 shows an example of this stabilization. This approach simulates a condensate accumulator as a stage with a larger holdup. To simulate complete distillation of the charge, the column draws on the boiler contents and holdups for top product, until the column is dry.

Without holdups, simulating a startup phase is not necessary. There is no

Figure 3-2 A Chain of Columns Integrating Batch Distillation

Neglecting Holdup

Accounting for Holdup

Figure 3-3. Stabilization of Holdup Compositions During Operation with Total Internal Reflux, for Test Case 1

inertia in a column without holdups, since the column starts each step empty.

Programs in this study simulated columns with and without holdups.

3.3 Performing Numerical Integration with a Flowsheet Simulator

Given: 1) the premise that a steady process model can simulate the instantaneous operation of a batch process, and 2) a means of evaluating the function, top product composition and flowrate as a function of bottom charge and heat rate, attention now turns to implementing its integration. Integration finds the function $y = y(P)$, where y is the product composition and P is the amount of product. Integration is necessary, because while distillate composition can be found from boiler composition, only the initial boiler composition is known and the process must be stepwise integrated to find the compositions at later times. The program integrates increments of product, and finds the residue composition as a function of them: $\int d(Lx) = \int d(Vy)$, as in the Rayleigh equation. This algorithm involves three issues: 1) evaluating and integrating the function in a general purpose process simulator (GPPS), 2) controlling stepsize, and 3) determining convergence.

This is the procedure for integration in a GPPS. The program feeds the initial charge and heat to a steady distillation modeling the batch still. It solves the column equations to predict the product compositions. These product flows and compositions for the initial instant of batch distillation are used to approximately predict the product over the first short interval, Δt , of the process.

Alternatively, the interval could be ΔP , a small amount of product, and the corresponding time interval could be calculated from energy balance and heat rate. The simulator calculates the charge remaining from the feed and product by material balance. This residue is the charge for the next interval of batch distillation and the feed for the next steady column simulating that batch distillation. What has just been described is a simple Euler integration of batch distillation: solving the differential equation by taking and integrating steps using the initial value of the slope in each interval. In this study, programs used this integration method.

The integration is easy, if tedious, to program in ASPEN PLUS. It is a chain of rectification columns, as shown in Figure 3-2. Each step of integration is a column, with its distillate going out of the flowsheet as a product and its bottoms feeding the column at the next step of integration. The program specifies the distillate flowrate, for example, and the raffinate flowrate decreases as the charge distills. The GPPS gives the results: distillate and raffinate compositions and flowrates, temperatures and heat rates for each column in the chain and hence for each step of integration. Appendix A contains an example of simulator output.

The program repeats the whole integration with smaller stepsizes until the result, distillate composition versus quantity distilled, is stable within a specified tolerance, that is, the integration has converged. Figure 3-4 shows an example

Figure 3-4. Convergence of QSSCA Simulation as Stepsize Shrinks
Accounting for Holdup in Test Cases 1 and 3

of this convergence. Since this is a first-order integration method, the difference between the results of one iteration and the ultimate converged solution decreases by a factor on the order of one half each time the stepsize halves (Riggs, 1988). Programming successive iterations with decreasing stepsizes requires human intervention, because process simulators currently cannot automatically change flowsheet arrangements (number of columns, connections, etc.), only process parameters (flowrates, temperatures, etc.). The programmer rewrites the flowsheet with, say, double the number of columns and half the stepsize and reruns the job. The rewriting and rerunning continue until the simulation converges. When the jobs are generated using a text editor, this is not nearly as tedious as it sounds.

Programs in this study were run with fixed-quantity stepsizes equaling 25%, 10%, 5%, 2.5%, 1% and 0.5% of the initial charge. This gave the visual demonstration of convergence in Figures 3-4 and 4-8. Examining these results suggests a more sophisticated algorithm for controlling integration stepsize. Distillate and raffinate compositions change slowly at the beginning, when the quantity of charge is large compared to the amount of distillate. These compositions change rapidly at the end, when distillate quantities become substantial fractions of the remaining charge. A stepsize small enough to accurately capture the end of the distillation curve wastes computer time in the beginning of distillation. To use computer time simulation. The engineer decides what sections of

the curve are important. For efficiency, stepsize should decrease during distillation. One way to do this is to make the distillate some fraction of the remaining charge at each step. The fractional approach needs a cut-off point, say 10% of original charge remaining or a crossover to a fixed quantity stepsize, because the simulation could go on forever, distilling the same percentage of the remaining charge.

A less visual and more mathematical convergence criterion could be some percentage variation in the accumulated product composition for the first quantity of distillate as the stepsize halves. Another criterion is convergence of amount distilled with some set purity. The convergence criterion derives from the purpose of the simulation. For example, the very end of the curve, which needs the smallest stepsize, probably does not need very close characterization, as the products and slop cuts have already distilled, and the bottom product simply is unloaded from the still pot. The program could separate the distillation into several separate problems. It could calculate each stage of the process with stepsize, convergence criteria and cutoff point appropriate for it. The approach is very flexible.

CHAPTER 4. TESTS, RESULTS and DISCUSSION

4.1 Description of the Tests

This chapter describes tests of the quasi-steady-state column approximation (QSSCA) approach in a specific application. The work of Domenech and Enjalbert (1974a,b) provides the information for the test cases, operating conditions and distillation curves. Table 4-1 lists their operating conditions, and Figure 4-1 shows their experimental and simulation results. They did a series of experiments to test the validity of their own rigorous fully dynamic (RFD) model. Domenech and Enjalbert batch distilled four mixtures of cyclohexane and toluene, a nonideal system. They used a pilot-scale column, and their experiments distilled about half the original charge. Several other investigators have tested their models against Domenech and Enjalbert's experiments. This gives an opportunity to compare this model with other models, and with experiments.

Table 4-1. Operating Conditions for Test Cases

<u>Initial Charge to Still</u>		<u>Distillation Column</u>		
Quantity	200 mol	Physical Stages	4 Sieve Trays	
Components	Cyclohexane (light) & Toluene	Stage Efficiency	75%	
Composition	Variable (see below)	Holdup	2.5 mol (on each tray and in the cond'r)	
		Condenser	Total	
		Reflux Ratio	Variable (see below)	
		Pressure	1 atm	
<u>Case Number</u>	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>
Reflux Ratio	3	4	6	5
Cyclohexane Charge	0.62	0.55	0.42	0.30

Figure 4-1. Domenech & Enjalbert's Results for Test Cases 1 thru 4
(Points are Experiments, Curves are RFD Simulations)

Exhibits 4-1, 4-2 and 4-3 and Appendix A are examples of the three-dimensional matrix of ASPEN PLUS programs written to cover the range of process models, step-sizes and process conditions. The programs display the three types of column models. Exhibit 4-2 and Appendix A show rigorous column calculations and accounting for liquid holdup on the trays. Because it accounts for holdup, the program in Exhibit 4-2 also includes simulation of column startup. The example program in Exhibit 4-1 also shows rigorous stage-by-stage calculations, but it neglects holdup. Exhibit 4-3 shows the Edmister overall column calculation. The program exhibits include columns simulating each step of distillation, and each program shows a different step-size. Exhibit 4-2 has 200 columns to simulate the 200 mol distillation in 1 mol steps, Exhibit 4-1 and Appendix A have four columns for 50 mol steps and Exhibit 4-3 has 20 columns for 10 mol product increments. Exhibit 4-2 includes seven columns producing no product overhead, to simulate convergence of the holdup compositions during startup. Each example implements the process conditions of one of Domenech and Enjalbert's tests. Exhibit 4-2 and Appendix A have specifications for Case 1, Exhibit 4-1 has Case 2, and Exhibit 4-3 has Case 4. Comments in the programs identify the specifications. The Methods Development Chapter discusses the principles behind the programs, including the startup simulation and interconnection between columns.

Exhibit 4-1. Program for QSSCA Simulation of Batch Distillation, Neglecting Holdup

TITLE "Batch Distillation Sim'n w/ QSSCA, Rigor Col Calc'n w/ No Holdup, 50mol/Step"
DESCRIPTION " Design & Operating Conditions for Domenech & Enjalbert's [D9,D11] Case 2"

IN-UNITS MET ;metric
OUT-UNITS MET

COMPONENTS C6H12 CYCLOHEXANE C6H12/ C7H8 TOLUENE C7H8
DATABANKS ASPENPCD ; ASPEN PLUS Component Data Bank
PROP-SOURCES ASPENPCD
PROPERTIES SYSOP7 ; UNIFAC/Redlich-Kwong

FLowsheet

; a free-standing column distilling 0.1mol to find composition of initial distillate
BLOCK 00DSTL IN=00FEED OUT=00TOPS 00BTMS

; chain of columns to integrate batch distillation in 50mol distillate steps

BLOCK 50DSTL IN=FEED OUT=50TOPS 50BTMS
BLOCK 100DSTL IN=50BTMS OUT=100TOPS 100BTMS
BLOCK 150DSTL IN=100BTMS OUT=150TOPS 150BTMS
BLOCK 199DSTL IN=150BTMS OUT=199TOPS 199BTMS

; distill 199 of 200 mols, to avoid errors when boiler runs dry

; feed streams are initial charges to batch boilers

STREAM 00FEED PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.200[KMOL/HR]
MOLE-FRAC C6H12 0.55/ C7H8 0.45 ; feed to column calc'ing initial distillate
STREAM FEED PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.200[KMOL/HR]
MOLE-FRAC C6H12 0.55/ C7H8 0.45 ; feed to chain of columns integrating batch
; atmospheric pressure and bubble-point temperature, D&E Case 2 compositions

; typical examples of unit operations blocks

BLOCK 00DSTL RADFRAC ; column calc'ing initial distillate
PARAM NSTAGE=6 EFF=MURPHREE
FEEDS 00FEED 6 ON-STAGE
PRODUCTS 00TOPS 1/ 00BTMS 6
P-SPEC 1 1[ATM]
COL-SPECS MOLE-RDV=0 MOLE-RR=4 MOLE-D=0.0001[KMOL/HR]
STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0

; chain of columns integrating batch

BLOCK 50DSTL RADFRAC ; rigorous fractionation calculation
PARAM NSTAGE=6 EFF=MURPHREE ; 6 stages=cond'r + 4 trays + boiler
FEEDS FEED 6 ON-STAGE ; charge to boiler=tray #6
PRODUCTS 50TOPS 1/ 50BTMS 6 ; TOPS=distillate product from tray #1,
; BTMS=boiler's remaining charge passed to the next column
P-SPEC 1 1[ATM] ; operating pressure
COL-SPECS MOLE-RDV=0 MOLE-RR=4 MOLE-D=0.050[KMOL/HR]
; total condenser => distillate vap/liq=0, molar reflux ratio=4, distillate=50mol/hr=stepsize
STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0 ; Murphree efficiencies

*

*

*

BLOCK 199DSTL RADFRAC ; last column in chain

Exhibit 4-2. Program for QSSCA Simulation of Batch Distillation, Accounting for Holdup

TITLE "Batch Distillation Sim'n w/ QSSCA, Rigor Col Calc'n w/ 2.5mol/tray Holdup, 1mol/Step"
DESCRIPTION " Design & Operating Conditions for Domenech & Enjalbert's [D9,D11] Case 1"

COMPONENTS C6H12 CYCLOHEXANE C6H12/ C7H8 TOLUENE C7H8
DATABANKS ASPENPCD ; ASPEN PLUS Component Data Bank
PROP-SOURCES ASPENPCD
PROPERTIES SYSOP7 ; UNIFAC/Redlich-Kwong

FLowsHEET ; chain of columns to startup and integrate batch distillation

```
; startup columns=0ADSTL thru 0FDSTL and 000DSTL, total internal reflux
BLOCK 0ADSTL IN=0AFEED1 0AFEED2 0AFEED3 0AFEED4 0AFEED5 0AFEED6 &
      OUT=0APROD1 0APROD2 0APROD3 0APROD4 0APROD5 0APROD6
BLOCK 0BDSTL IN=0APROD1 0APROD2 0APROD3 0APROD4 0APROD5 0APROD6 &
      OUT=0BPROD1 0BPROD2 0BPROD3 0BPROD4 0BPROD5 0BPROD6
; sidestreams=0APROD1, 0APROD2,...,0APROD5, 0APROD6, from condenser, top tray,
; ...,bottom tray and boiler, respectively, are holdups passed from column to column.
*
BLOCK 000DSTL IN=0FPROD1 0FPROD2 0FPROD3 0FPROD4 0FPROD5 0FPROD6 &
      OUT=000PROD1 000PROD2 000PROD3 000PROD4 000PROD5 000PROD6

; production columns=001DSTL thru 200DSTL, producing 1mol/col distillate
BLOCK 001DSTL IN=000PROD1 000PROD2 000PROD3 000PROD4 000PROD5 000PROD6 &
      OUT=001PROD1 001PROD2 001PROD3 001PROD4 001PROD5 001PROD6
BLOCK 001SPLT IN=001PROD1   OUT=002FEED1 Z001TOPS

BLOCK 002DSTL IN=002FEED1 001PROD2 001PROD3 001PROD4 001PROD5 001PROD6 &
      OUT=002PROD1 002PROD2 002PROD3 002PROD4 002PROD5 002PROD6
BLOCK 002SPLT IN=002PROD1   OUT=003FEED1 Z002TOPS
*
BLOCK 200DSTL IN=200FEED1 199PROD2 199PROD3 199PROD4 199PROD5 199PROD6 &
      OUT=200PROD1 200PROD2 200PROD3 200PROD4 200PROD5 200PROD6
BLOCK 200SPLT IN=200PROD1   OUT=201FEED1 Z00TOPS

; feed streams=initial holdups fed to cond'r and trays=0.0025[kmol],
; and remainder charged to boiler=200-12.5=0.01875[kmol].
; atmospheric pressure, bubble-point temperature, D&E Case 1 compositions

STREAM 0AFEED1 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL/HR]
MOLE-FRAC C6H12 0.62/ C7H8 0.38
STREAM 0AFEED2 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL/HR]
MOLE-FRAC C6H12 0.62/ C7H8 0.38
*
STREAM 0AFEED6 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.1876[KMOL/HR]
MOLE-FRAC C6H12 0.62/ C7H8 0.38
```

Exhibit 4-2. Program for QSSCA Simulation of Batch Distillation, Accounting for Holdup (continued)

```

; typical examples of unit operations blocks

; startup columns=0ADSTL thru 0FDSTL and 000DSTL, total internal reflux
BLOCK 0ADSTL RADFRAC ; rigorous fractionation calculationn
PARAM NSTAGE=6 EFF=MURPHREE ; 6 stages=cond'r + 4 trays + boiler
; holdup feeds to condenser and trays, and charge to boiler
FEEDS 0AFEED1 1 ON-STAGE/ & ; condenser (top of column)
      0AFEED2 2 ON-STAGE/ & ; 1st tray
      0AFEED3 3 ON-STAGE/ & ; 2nd tray
      0AFEED4 4 ON-STAGE/ & ; 3rd tray
      0AFEED5 5 ON-STAGE/ & ; 4th tray
      0AFEED6 6 ON-STAGE ; boiler (btm of column)
; liquid holdup products from condenser, trays and boiler
PRODUCTS 0APROD1 1/ & ; cond'r's phase=l & flow=.0025 set in COL-SPECS
        0APROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        0APROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        0APROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        0APROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        0APROD6 6 ; boiler's holdup is its charge to the next column
P-SPEC 1 1[ATM] ; operating pressure
COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
; total condenser => distillate vap/liq=0, molar reflux ratio=3,
; distillate=0.0025[kmol/col]=condenser's holdup product
STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0 ; Murphree efficiencies

; production columns=001DSTL thru 200DSTL, producing 1[mol/hr-col] distillate
BLOCK 001DSTL RADFRAC ; typical production column
PARAM NSTAGE=6 EFF=MURPHREE
FEEDS 000PROD1 1 ON-STAGE/ &
      000PROD2 2 ON-STAGE/ &
      000PROD3 3 ON-STAGE/ &
      000PROD4 4 ON-STAGE/ &
      000PROD5 5 ON-STAGE/ &
      000PROD6 6 ON-STAGE
PRODUCTS 001PROD1 1/ &
        001PROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        001PROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        001PROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        001PROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
        001PROD6 6
P-SPEC 1 1[ATM]
COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0035[KMOL/HR]
STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0

BLOCK 001SPLT FSPLIT
MOLE-FLOW 002FEED1 0.0025[KMOL/HR]
; 001PROD1=0.0035[kmol/col]=distillate, is split between
; 002FEED1=0.0025[kmol/col]=cond'r holdup to next column, and
; Z001TOPS=0.0010[kmol/col]=product

```

Exhibit 4-3. Program for QSSCA Simimulation of Batch Distillation, Shortcut Column Calculation

TITLE "Batch Distillation Sim'n w/ QSSCA, Shortcut Col Calc'n w/ No Holdup, 10mol/Step"
DESCRIPTION " Design & Operating Conditions for Domenech & Enjalbert's [D9,D11] Case 4"

IN-UNITS MET ;metric
OUT-UNITS MET
COMPONENTS C6H12 CYCLOHEXANE C6H12/ C7H8 TOLUENE C7H8
DATABANKS ASPENPCD ; ASPEN PLUS Component Data Bank
PROP-SOURCES ASPENPCD
PROPERTIES SYSOP7 ; UNIFAC/Redlich-Kwong

FLWSHEET ; chain of columns to integrate batch distillation in 10mol distillate steps

BLOCK 000DSTL IN=FEED	OUT=Z000TOPS 000BTMS
BLOCK 010DSTL IN=000BTMS	OUT=Z010TOPS 010BTMS
BLOCK 020DSTL IN=010BTMS	OUT=Z020TOPS 020BTMS

*
*
*

BLOCK 190DSTL IN=180BTMS	OUT=Z190TOPS 190BTMS
BLOCK 200DSTL IN=190BTMS	OUT=Z200TOPS 200BTMS

; shortcut columns have one feed and two outputs: TOPS=distillate product
; and BTMS=remaining charge fed to next column

; feed stream is initial charges to first batch boiler
STREAM FEED PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-
FLOW=0.200[KMOL/HR]
MOLE-FRAC C6H12 0.30/ C7H8 0.70 ; for RR=5
; atmospheric pressure and bubble-point temperature, D&E Case 4 compositions

;typical examples of unit operations blocks

BLOCK 000DSTL DISTL ; first column distills 0.002mol to find initial distillate composition
PARAM NSTAGE=5 FEED-LOC=5 RR=5 D:F=0.00001 & ;
distill/feed=.002mol/200mol
COND-TYPE=TOTAL PTOP=1[ATM] PBOT=1[ATM]

BLOCK 010DSTL DISTL ; edmister shortcut column calculation
PARAM NSTAGE=5 FEED-LOC=5 RR=5 D:F=0.05 &
COND-TYPE=TOTAL PTOP=1[ATM] PBOT=1[ATM]
; column has 5 stages (incl. boiler) plus total cond'r, feed to stage 5=btm=boiler
; reflux ratio=5, distillate/feed=0.05=10mol/200mol, 1atm oper. pressure

BLOCK 020DSTL DISTL
PARAM NSTAGE=5 FEED-LOC=5 RR=5 D:F=0.05263 & ;
distill/feed=10mol/190mol
COND-TYPE=TOTAL PTOP=1[ATM] PBOT=1[ATM]

*
*
*

BLOCK 190DSTL DISTL
PARAM NSTAGE=5 FEED-LOC=5 RR=5 D:F=0.5 & ; distill/feed=10mol/20mol
COND-TYPE=TOTAL PTOP=1[ATM] PBOT=1[ATM]

BLOCK 200DSTL DISTL ; last col distills 9.9999 of 10mol remaining, to avoid error
PARAM NSTAGE=5 FEED-LOC=5 RR=5 D:F=0.99999 &
COND-TYPE=TOTAL PTOP=1[ATM] PBOT=1[ATM]

4.2 Results and Discussion

All the simulations ran with no errors. In some simulations, all of the light component went overhead before the boiler was empty. When this occurred, ASPEN PLUS issued warnings objecting to continuing distillation with only one component. This warning did not indicate a real problem. All the results were rational: mol fractions between 0 and 1, flowrates positive, etc. ASPEN PLUS's calculations of its unit operations models, mostly distillation columns all converged. The runs were stable. As simulation and process parameters changed, the results changed in reasonable ways, not showing excessive sensitivity or blowing-up.

Running these ASPEN PLUS programs to simulate the test cases generated voluminous output. Distillation curve data were extracted from the output. Some are shown in this chapter and Chapter 3, and all are collected in Appendix B. Appendix A contains a short example of ASPEN PLUS output.

Besides being "computer correct," the results make "chemical engineering sense." All unit operations and overall flowsheets are in material and energy balance (Appendix A). The more volatile component, cyclohexane, distills above the less volatile, toluene. Figure 4-2 shows that the light component concentration increases, and the heavy component concentration decreases along the column from boiler to condenser, throughout the distillation. Following the distillate composition over time in Figure 4-3, all simulations show a plateau of cyclohexane, which falls off as it distills away and toluene begins distilling. The

Figure 4-2. Variation of Light Component along the Column in QSSCA Simulation of Test Case 2, with Holdup and 20mol Steps

Figure 4-3. QSSCA Simulation Curves for Test Cases 1 thru 4
(Simulating Holdup and Integrating in 1 mol Steps)

simulations respond to changes in process conditions as distillations normally do. When the initial charge to the boiler is richer in the light component, the first distillate is richer in it too. Comparing Cases 1 and 2 with Cases 3 and 4 in Figure 4-3 shows this. When the reflux ratio is higher, the break in the distillation curve after the light plateau is sharper. Comparing Case 3 with Case 4 demonstrates this. These comparisons are not as clear-cut as one might wish, because the boiler charge and the reflux ratio vary simultaneously in these tests.

Figures 4-4 and 4-5 compare published simulations and simulations from this study against experimental data. Domenech and Enjalbert's model uses a fully dynamic approach. Its predictions are in excellent accord with their experimental results. Galindez and Fredenslund's (1988b) model uses QSSCA. Its predictions capture the shapes of the distillation curves, and predict the distillate accumulations when the curves break. However, its distillate cyclohexane predictions are a bit too high during the first part of distillation, before the break. This study's simulation, using a similar model, gives similar results. In Cases 1 and 2, its predictions follow the cyclohexane plateaus well, and simulate the curves' breaks almost as well as Galindez and Fredenslund's model. In Cases 3 and 4, its predictions follow the plateaus more closely than Galindez and Fredenslund's model; after the break both models give equally good, though not identical, predictions of the curves. Both this simulation and Galindez and Fredenslund's simulation predict the cyclohexane plateau too high. This could be due to many factors, including inexact correspondence between the physical

Figure 4-4. Comparison of Published Simulations for
for Test Cases 1 and 3 (QSSCA Sim'n taking 1 mol Steps)

Figure 4-5. Comparison of Published Simulations for
for Test Cases 2 and 4 (QSSCA Sim'n taking 1 mol Steps)

properties model and the actual chemical system. In both simulations, the over-prediction of the plateau increases as reflux ratio increases; this is most clearly seen by comparing Cases 1 and 3, with reflux ratios of 3 and 6, in Figure 4-4. This trend could be the result of using a constant stage efficiency of 75%. The efficiency could decrease as vapor and liquid flowrates increases with the reflux ratio. Decreasing efficiency would degrade separation and lower the cyclohexane plateau.

Chiotti and Scenna's (1989) model also uses QSSCA, but, unlike Galindez and Fredenslund's, it neglects holdup. The agreement of their model's predictions with experimental results is poorer than that of Domenech and Enjalbert's or Galindez and Fredenslund's models. During the first part of the distillation, it predicts distillate cyclohexane values that are far too high. With material balance, these high values cause it to predict the break in the distillation curve far too early. This is true in Cases 1, 2, 3; they did not publish predictions for Case 4. Diwekar and Madhavan's (1991c) model uses QSSCA with a short-cut column calculation; other models employ plate-to-plate column calculations. The accuracy of its predictions varies in Cases 2, 3 and 4; they did not report on Case 1. In Case 2, it predicts the early distillate quite well, but it predicts the break from the plateau too early. It predicts the plateau too high in Case 3. In Case 4, its predictions follow the experimental points closely. Overall, this study's model compares quite favorably with those in the literature.

These results suggest that simplifying the model degrades the accuracy of its predictions. The correlation of complexity and accuracy in the literature is only a correlation. The literature contains different models by different investigators, so factors besides complexity may be at work. Published accounts lack sufficient detail to identify and control for these factors. In the work reported here, these extraneous factors are under control, and examining the complexity and accuracy relationship should be possible. Figures 4-6 and 4-7 compare converged simulations by the three column models. The simplest model, which uses short-cut column calculations, gives the poorest predictions. However, the most complex model, which does plate-to-plate column calculations and accounts for holdup, does no better than the simpler model, which calculates plate-to-plate but neglects holdup. Thus, this study's results are ambiguous on the complexity and accuracy relationship, probably because holdup can be neglected in these cases.

Publications generally report only the final converged results of a model. They seldom report on convergence behavior. This work retains that information and discusses it. Figures 3-3 and 4-8 show the behavior of the simulations as distillate step-size decreases. As step-size decreases from 50 to 20 to . . . to 2 to 1 mol out of a 200 mol batch, the simulations show no signs of instability. At all points along their lengths, the difference between successive distillation curves decreases as step-size decreases, and they converge toward a final result. Aside from small differences, the three column models show similar be-

Figure 4-6. Effect of Column Model on QSSCA Simulation of Test Cases 1 and 3 (Integrating with 1 mol Steps)

Figure 4-7. Effect of Column Model on QSSCA Simulation of Test Cases 2 and 4 (Integrating with 1 mol Steps)

Figure 4-8. Convergence of QSSCA Simulation as Stepsize Shrinks
Accounting for Holdup in Test Cases 2 and 4

havior in all four cases. As the curves converge, they do not always converge to their best agreement with the experimental results. During the light component plateau before the break, the No Holdup and Short-Cut simulations converge down to better agreement with the experimental points. The Holdup simulation converges slightly upward and away from the experiment during this period, though its shape improves. After the break, all the simulation curves drop below Domenech and Enjalbert's last few points as they converge. The break sharpens as the step-size decreases.

CHAPTER 5. CONCLUSIONS on HYPOTHESES

Chapter 1 states the motivations for this investigation: the importance of batch distillation, the necessity for process simulation in batch column design, and the shortcomings of existing simulation software. It finds "an unmet need for an easy procedure for implementing batch distillation simulation using the quasi-steady-state column approximation (QSSCA) in a widely available flowsheet simulator." This finding leads to the research objective: "to develop and investigate a straightforward implementation of the quasi-steady-state column approximation approach to batch distillation simulation on a commercial modular process simulator." To achieve this objective, this study investigated three hypotheses. This section will summarize the conclusions of this investigation.

The first and third hypotheses are:

"A batch distillation simulation based on the QSSCA approach can be implemented on a prototypical, commercial, modular process simulator."

"A general paradigm can be illustrated to facilitate implementation of this simulation technique."

The Methods Development and Results Chapters demonstrate the truth of these hypotheses. Chapter 3 justifies the QSSCA approach with a discussion of how a steady-state model can simulate a batch process over a short interval. Step 1 in Exhibit 5-1 summarizes general principles for creating a steady column model simulating a batch distillation column. Using this facility for simulating intervals of

batch distillation, Chapter 3 describes how to integrate these intervals to predict the distillate and raffinate compositions and volumes during distillation. This involves a chain of columns, one for each step-of-integration, where the bottoms and holdups of one column are the feeds to the next. The numerical integration is converged by adding columns to the chain, to decrease the size of the intervals, until the results are not changing by more than a specified tolerance. The simulation is programmed first with short-cut column calculations and neglecting column holdup and then with rigorous column calculations, neglecting and accounting for holdup. The results are compared to determine if there is a significant difference which justifies the more rigorous approach. Table 5-1 summarizes the procedure above. Development of general criteria determining which processes need the rigorous approach and which can use short-cut calculations is beyond the scope of this study. This determination can be done on a case-by-case basis by engineers using this procedure.

These principles have been applied before, for example the freestanding programs of Galindez and Fredenslund (1988b), and Diwekar and Madhavan (1991c). This study extends this work, applying this approach within the environment of a general purpose process simulator (GPPS). Chapters 3 and 4 describe how to apply these principles to translate Domenech and Enjalbert's description of batch distillation experiments (1974a,b) into a model in ASPEN PLUS. Domenech and Enjalbert's batch column is not atypical, and the ASPEN PLUS program uses only the primary commands available in the simulation language,

no tricks or custom FORTRAN modules. Therefore the paradigm should be quite general, and allow simulation of many batch columns for which a GPPS can provide a steady column model. However widely applicable, this approach surely will not be universal. Therefore, in each new application, the user must independently assess the accuracy of its predictions before using them for design.

The second hypothesis is "Results from this simulator are comparable with the results of published simulations using the QSSCA approach." In Chapter 4 and Appendices A and B, the test results demonstrate the success of this simulator. It runs correctly, according to both mathematical and chemical engineering criteria, and it closely approximates experimental batch distillation curves. Its performance is better than that of Chiotti and Scenna's (1989), and Diwekar and Madhavan's (1991c) simple QSSCA simulations, and comparable to Galindez and Fredenslund's sophisticated QSSCA simulation (1988b). However, it is not as accurate as the rigorous fully dynamic (RFD) simulation of Domenech and Enjalbert (1974a,b). This performance leads to the recommendation to use QSSCA with short-cut models for preliminary design scouting, use QSSCA with rigorous columns to optimize, and use RFD simulation to check the final design and investigate process control. All of this can be done in the same process simulator environment, using the techniques developed in this thesis.

Exhibit 5-1. Procedure for Simulating Batch Distillation with a Steady Column in a General Purpose Process Simulator

- 1) Formulate a steady column model of the batch column according to the principles developed in Chapter 3.
 - a) Over the time interval being modeled, the feed to the steady process must equal the quantity and composition of the initial inventory in the batch process. For example, 100 kg/hour feed to a steady process to model batch processing of 100 kg for one hour.
 - b) The heat and distillate production rates in the steady and batch processes should be equal.
 - c) The steady and batch processes should have the same column design (number of stages, stage efficiency, operating pressure, etc.).
 - d) Holdups in the batch column should be simulated as stage feeds and products in the steady column model as described by Galindez and Fredenslund.
 - e) Holdups should be established in the steady column by simulating operation with total internal reflux before distillate production begins.
- 2) Program the flowsheet simulator for the steady column model.
- 3) Run the simulation and correct the inevitable programming errors.
- 4) Divide the batch distillation into intervals and add a steady column model for each interval to integrate the simulation over the whole process
- 5) Run the integrating simulation. Check the results with chemical engineering logic to be sure that they are reasonable. Compare the results with experiments, if possible.
- 6) Decrease the interval size and re-run the simulation until it has converged.
- 7) Use short-cut column calculations and neglect column holdup in the simulation procedure described above.
- 8) Use rigorous column calculations, neglecting and accounting for column holdup in the simulation.
- 9) Compare the three results to determine if there is a significant difference which justifies the more rigorous approach.

APPENDIX A. EXAMPLE OF SIMULATOR OUTPUT

This example was generated by running the program 50D3RHU.INP in ASPEN PLUS by the command: "ASPEN 50D3RHU.INP 50D3RHU." After the run, ASPEN PLUS's history and report files were combined into an output file with the command: "GENOUT 50D3RHU."

ASPENTECH
 FLOWSHEET SIMULATION
 FOR THE PROCESS INDUSTRIES

AAAAA	SSSSS	PPPPP	EEEE	NN	N	PPPPP	L	U	U	SSSSS	TM		
A	A	S	P	P	E	N	N	P	P	L	U	U	S
AAAAA	SSSSS	PPPPP	EEEE	N	N	N	PPPPP	L	U	U	SSSSS		
A	A	S	P	E	N	NN	P	L	U	U	S		
A	A	SSSSS	P	EEEE	N	N	P	LLLLL	UUUUU	SSSSS			

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 EUROPE 31-70-3541051

VERSION: DOS-386
 RELEASE: 8.4-1
 INSTALLATION: sjsu-utv

JANUARY 4, 1993
 MONDAY
 8:31:00 A.M.

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*** INPUT ECHO(ES) ***

>>CURRENT RUN

ORIGINAL RUN
8:31:00 A.M.
INPUT FILE: 50D3RHUR.inp
OUTPUT PDF: 50D3RHUR VERSION: 1
LOCATED IN: E:\CHE_STOK\CHEXANE\HOLDUP\50D3RHUR
PDF SIZE: FILE (PSIZE)=99999 RECORDS. IN-CORE = 2000 RECORDS.

JANUARY 4, 1993
MONDAY

```
1  TITLE " D&E 74, RR=3: 50KMOL/Col, HOLDUP, MEff'cy=0.75 "
2  RUN-CONTROL  MAX-TIME=10000  MAX-ERRORS=100
3
4  IN-UNITS MET
5  OUT-UNITS MET
6  BLOCK-REPORT NOSORT
7  STREAM-REPORT NOSORT
8
9  COMPONENTS  C6H12 CYCLOHEXANE C6H12/  C7H8 TOLUENE C7H8
10 DATABASES  ASPENPCD
11 PROP-SOURCES  ASPENPCD
12 PROPERTIES  SYSOP7
13
14 FLOWSHEET
15
16  BLOCK  OADSTL  IN=0AFEED1  0AFEED2  0AFEED3  0AFEED4  0AFEED5  0AFEED6
17  OUT=0APROD1  0APROD2  0APROD3  0APROD4  0APROD5  0APROD6
18
19  BLOCK  OBDSTL  IN=0APROD1  0APROD2  0APROD3  0APROD4  0APROD5  0APROD6
20  OUT=0BPROD1  0BPROD2  0BPROD3  0BPROD4  0BPROD5  0BPROD6
21
22  BLOCK  OCDSTL  IN=0BPROD1  0BPROD2  0BPROD3  0BPROD4  0BPROD5  0BPROD6
23  OUT=0CPROD1  0CPROD2  0CPROD3  0CPROD4  0CPROD5  0CPROD6
24
25  BLOCK  ODDSTL  IN=0CPROD1  0CPROD2  0CPROD3  0CPROD4  0CPROD5  0CPROD6
26  OUT=0DPROD1  0DPROD2  0DPROD3  0DPROD4  0DPROD5  0DPROD6
27
28  BLOCK  OEDSTL  IN=0DPROD1  0DPROD2  0DPROD3  0DPROD4  0DPROD5  0DPROD6
29  OUT=0EPROD1  0EPROD2  0EPROD3  0EPROD4  0EPROD5  0EPROD6
30
31  BLOCK  OFDSTL  IN=0EPROD1  0EPROD2  0EPROD3  0EPROD4  0EPROD5  0EPROD6
32  OUT=0FPROD1  0FPROD2  0FPROD3  0FPROD4  0FPROD5  0FPROD6
33
34  BLOCK  O00DSTL  IN=0FPROD1  0FPROD2  0FPROD3  0FPROD4  0FPROD5  0FPROD6
35  OUT=000PROD1  000PROD2  000PROD3  000PROD4  000PROD5  000PROD6
36
37  BLOCK  O50DSTL  IN=000PROD1  000PROD2  000PROD3  000PROD4  000PROD5  000PROD6
38  OUT=050PROD1  050PROD2  050PROD3  050PROD4  050PROD5  050PROD6
39  BLOCK  O50SPLT  IN=050PROD1  OUT=100FEED1  Z050TOPS
40
41  BLOCK  100DSTL  IN=100FEED1  050PROD2  050PROD3  050PROD4  050PROD5  050PROD6
42  OUT=100PROD1  100PROD2  100PROD3  100PROD4  100PROD5  100PROD6
43  BLOCK  100SPLT  IN=100PROD1  OUT=150FEED1  Z100TOPS
44
45  BLOCK  150DSTL  IN=150FEED1  100PROD2  100PROD3  100PROD4  100PROD5  100PROD6
46  OUT=150PROD1  150PROD2  150PROD3  150PROD4  150PROD5  150PROD6
47  BLOCK  150SPLT  IN=150PROD1  OUT=200FEED1  Z150TOPS
48
49  BLOCK  200DSTL  IN=200FEED1  150PROD2  150PROD3  150PROD4  150PROD5  150PROD6
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50      OUT=200PROD1 200PROD6
51      BLOCK 200SPLT IN=200PROD1      OUT=250FEED1 Z200TOPS
52
53      ; Streams and Unit Operation Blocks
54
55      STREAM OAFEED1 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL
56      MOLE-FRAC C6H12 0.62/ C7H8 0.38
57      STREAM OAFEED2 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL
58      MOLE-FRAC C6H12 0.62/ C7H8 0.38
59      STREAM OAFEED3 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL
60      MOLE-FRAC C6H12 0.62/ C7H8 0.38
61      STREAM OAFEED4 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL
62      MOLE-FRAC C6H12 0.62/ C7H8 0.38
63      STREAM OAFEED5 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.00250[KMOL
64      MOLE-FRAC C6H12 0.62/ C7H8 0.38
65      STREAM OAFEED6 PRES=1[ATM] VFRAC=0 NPHASE=2 MOLE-FLOW=0.1876[KMOL/
66      MOLE-FRAC C6H12 0.62/ C7H8 0.38
67      ; Atmospheric Pressure and Bubble-point Temperature,
68      ; Flow/Batch and Conc'n from Galendez & Fredenslund, 1988, p.287
69
70      BLOCK OADSTL RADFRAC
71      PARAM NSTAGE=6 EFF=MURPHREE
72      FEEDS OAFEED1 1 ON-STAGE/ &
73      OAFEED2 2 ON-STAGE/ &
74      OAFEED3 3 ON-STAGE/ &
75      OAFEED4 4 ON-STAGE/ &
76      OAFEED5 5 ON-STAGE/ &
77      OAFEED6 6 ON-STAGE
78      PRODUCTS OAPROD1 1/ &
79      OAPROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
80      OAPROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
81      OAPROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
82      OAPROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
83      OAPROD6 6
84      P-SPEC 1 1[ATM]
85      COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
86      STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
87
88      BLOCK OBDSTL RADFRAC
89      PARAM NSTAGE=6 EFF=MURPHREE
90      FEEDS OAPROD1 1 ON-STAGE/ &
91      OAPROD2 2 ON-STAGE/ &
92      OAPROD3 3 ON-STAGE/ &
93      OAPROD4 4 ON-STAGE/ &
94      OAPROD5 5 ON-STAGE/ &
95      OAPROD6 6 ON-STAGE
96      PRODUCTS OBPROD1 1/ &
97      OBPROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
98      OBPROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
99      OBPROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
100     OBPROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
101     OBPROD6 6
102     P-SPEC 1 1[ATM]
103     COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
104     STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
105
106     BLOCK OCDSTL RADFRAC
107     PARAM NSTAGE=6 EFF=MURPHREE
108     FEEDS OBPROD1 1 ON-STAGE/ &
109     OBPROD2 2 ON-STAGE/ &

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110          OBPROD3 3 ON-STAGE/ &
111          OBPROD4 4 ON-STAGE/ &
112          OBPROD5 5 ON-STAGE/ &
113          OBPROD6 6 ON-STAGE
114  PRODUCTS  OCPROD1 1/ &
115          OCPROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
116          OCPROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
117          OCPROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
118          OCPROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
119          OCPROD6 6
120  P-SPEC 1 1[ATM]
121  COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
122  STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
123
124  BLOCK ODDSTL RADFRAC
125  PARAM NSTAGE=6 EFF=MURPHREE
126  FEEDS  OCPROD1 1 ON-STAGE/ &
127          OCPROD2 2 ON-STAGE/ &
128          OCPROD3 3 ON-STAGE/ &
129          OCPROD4 4 ON-STAGE/ &
130          OCPROD5 5 ON-STAGE/ &
131          OCPROD6 6 ON-STAGE
132  PRODUCTS ODPROD1 1/ &
133          ODPROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
134          ODPROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
135          ODPROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
136          ODPROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
137          ODPROD6 6
138  P-SPEC 1 1[ATM]
139  COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
140  STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
141
142  BLOCK OEDSTL RADFRAC
143  PARAM NSTAGE=6 EFF=MURPHREE
144  FEEDS  ODPROD1 1 ON-STAGE/ &
145          ODPROD2 2 ON-STAGE/ &
146          ODPROD3 3 ON-STAGE/ &
147          ODPROD4 4 ON-STAGE/ &
148          ODPROD5 5 ON-STAGE/ &
149          ODPROD6 6 ON-STAGE
150  PRODUCTS OEPROD1 1/ &
151          OEPROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
152          OEPROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
153          OEPROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
154          OEPROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
155          OEPROD6 6
156  P-SPEC 1 1[ATM]
157  COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
158  STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
159
160  BLOCK OFDSTL RADFRAC
161  PARAM NSTAGE=6 EFF=MURPHREE
162  FEEDS  OEPROD1 1 ON-STAGE/ &
163          OEPROD2 2 ON-STAGE/ &
164          OEPROD3 3 ON-STAGE/ &
165          OEPROD4 4 ON-STAGE/ &
166          OEPROD5 5 ON-STAGE/ &
167          OEPROD6 6 ON-STAGE
168  PRODUCTS OFPROD1 1/ &
169          OFPROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &

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170          OFPROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
171          OFPROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
172          OFPROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
173          OFPROD6 6
174 P-SPEC 1 1[ATM]
175 COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
176 STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
177
178 BLOCK 000DSTL RADFRAC
179 PARAM NSTAGE=6 EFF=MURPHREE
180 FEEDS OFPROD1 1 ON-STAGE/ &
181       OFPROD2 2 ON-STAGE/ &
182       OFPROD3 3 ON-STAGE/ &
183       OFPROD4 4 ON-STAGE/ &
184       OFPROD5 5 ON-STAGE/ &
185       OFPROD6 6 ON-STAGE
186 PRODUCTS 000PROD1 1/ &
187          000PROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
188          000PROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
189          000PROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
190          000PROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
191          000PROD6 6
192 P-SPEC 1 1[ATM]
193 COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0025[KMOL/HR]
194 STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
195
196 BLOCK 050DSTL RADFRAC
197 PARAM NSTAGE=6 EFF=MURPHREE
198 FEEDS 000PROD1 1 ON-STAGE/ &
199       000PROD2 2 ON-STAGE/ &
200       000PROD3 3 ON-STAGE/ &
201       000PROD4 4 ON-STAGE/ &
202       000PROD5 5 ON-STAGE/ &
203       000PROD6 6 ON-STAGE
204 PRODUCTS 050PROD1 1/ &
205          050PROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
206          050PROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
207          050PROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
208          050PROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
209          050PROD6 6
210 P-SPEC 1 1[ATM]
211 COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0525[KMOL/HR]
212 STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
213
214 BLOCK 050SPLT FSPLIT
215 MOLE-FLOW 100FEED1 0.0025[KMOL/HR]
216
217 BLOCK 100DSTL RADFRAC
218 PARAM NSTAGE=6 EFF=MURPHREE
219 FEEDS 100FEED1 1 ON-STAGE/ &
220       050PROD2 2 ON-STAGE/ &
221       050PROD3 3 ON-STAGE/ &
222       050PROD4 4 ON-STAGE/ &
223       050PROD5 5 ON-STAGE/ &
224       050PROD6 6 ON-STAGE
225 PRODUCTS 100PROD1 1/ &
226          100PROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
227          100PROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
228          100PROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
229          100PROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &

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230          100PROD6 6
231 P-SPEC 1 1[ATM]
232 COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0525[KMOL/HR]
233 STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
234
235 BLOCK 100SPLT FSPLIT
236 MOLE-FLOW 150FEED1 0.0025[KMOL/HR]
237
238 BLOCK 150DSTL RADFRAC
239 PARAM NSTAGE=6 EFF=MURPHREE
240 FEEDS 150FEED1 1 ON-STAGE/ &
241 100PROD2 2 ON-STAGE/ &
242 100PROD3 3 ON-STAGE/ &
243 100PROD4 4 ON-STAGE/ &
244 100PROD5 5 ON-STAGE/ &
245 100PROD6 6 ON-STAGE
246 PRODUCTS 150PROD1 1/ &
247 150PROD2 2 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
248 150PROD3 3 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
249 150PROD4 4 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
250 150PROD5 5 PHASE=L MOLE-FLOW=0.0025[KMOL/HR]/ &
251 150PROD6 6
252 P-SPEC 1 1[ATM]
253 COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.0525[KMOL/HR]
254 STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
255
256 BLOCK 150SPLT FSPLIT
257 MOLE-FLOW 200FEED1 0.0025[KMOL/HR]
258
259 BLOCK 200DSTL RADFRAC
260 PARAM NSTAGE=6 EFF=MURPHREE
261 FEEDS 200FEED1 1 ON-STAGE/ &
262 150PROD2 2 ON-STAGE/ &
263 150PROD3 3 ON-STAGE/ &
264 150PROD4 4 ON-STAGE/ &
265 150PROD5 5 ON-STAGE/ &
266 150PROD6 6 ON-STAGE
267 PRODUCTS 200PROD1 1/ &
268 200PROD6 6
269 P-SPEC 1 1[ATM]
270 COL-SPECS MOLE-RDV=0 MOLE-RR=3 MOLE-D=0.050[KMOL/HR]
271 STAGE-EFF 1 1.0/ 2 0.75/ 3 0.75/ 4 0.75/ 5 0.75/ 6 1.0
272
273 BLOCK 200SPLT FSPLIT
274 MOLE-FLOW 250FEED1 0.000[KMOL/HR]
275
*** INPUT TRANSLATOR MESSAGES ***

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THIS VERSION OF ASPEN PLUS LICENSED TO SAN JOSE STATE UNIVERSITY

*** FLOWSHEET ANALYSIS MESSAGES ***

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
0AFEED6	----	0ADSTL	0AFEED5	----	0ADSTL
0AFEED4	----	0ADSTL	0AFEED3	----	0ADSTL
0AFEED2	----	0ADSTL	0AFEED1	----	0ADSTL
0APROD1	0ADSTL	0BDSTL	0APROD2	0ADSTL	0BDSTL

0APROD3	0ADSTL	0BDSTL	0APROD4	0ADSTL	0BDSTL
0APROD5	0ADSTL	0BDSTL	0APROD6	0ADSTL	0BDSTL
0BPROD1	0BDSTL	0CDSTL	0BPROD2	0BDSTL	0CDSTL
0BPROD3	0BDSTL	0CDSTL	0BPROD4	0BDSTL	0CDSTL
0BPROD5	0BDSTL	0CDSTL	0BPROD6	0BDSTL	0CDSTL
0CPROD1	0CDSTL	0DDSTL	0CPROD2	0CDSTL	0DDSTL
0CPROD3	0CDSTL	0DDSTL	0CPROD4	0CDSTL	0DDSTL
0CPROD5	0CDSTL	0DDSTL	0CPROD6	0CDSTL	0DDSTL
0DPROD1	0DDSTL	0EDSTL	0DPROD2	0DDSTL	0EDSTL
0DPROD3	0DDSTL	0EDSTL	0DPROD4	0DDSTL	0EDSTL
0DPROD5	0DDSTL	0EDSTL	0DPROD6	0DDSTL	0EDSTL
0EPROD1	0EDSTL	0FDSTL	0EPROD2	0EDSTL	0FDSTL
0EPROD3	0EDSTL	0FDSTL	0EPROD4	0EDSTL	0FDSTL
0EPROD5	0EDSTL	0FDSTL	0EPROD6	0EDSTL	0FDSTL
0FPROD1	0FDSTL	000DSTL	0FPROD2	0FDSTL	000DSTL
0FPROD3	0FDSTL	000DSTL	0FPROD4	0FDSTL	000DSTL
0FPROD5	0FDSTL	000DSTL	0FPROD6	0FDSTL	000DSTL
000PROD1	000DSTL	050DSTL	000PROD2	000DSTL	050DSTL
000PROD3	000DSTL	050DSTL	000PROD4	000DSTL	050DSTL
000PROD5	000DSTL	050DSTL	000PROD6	000DSTL	050DSTL
050PROD1	050DSTL	050SPLT	050PROD2	050DSTL	100DSTL
050PROD3	050DSTL	100DSTL	050PROD4	050DSTL	100DSTL
050PROD5	050DSTL	100DSTL	050PROD6	050DSTL	100DSTL
100FEED1	050SPLT	100DSTL	Z050TOPS	050SPLT	----
100PROD1	100DSTL	100SPLT	100PROD2	100DSTL	150DSTL
100PROD3	100DSTL	150DSTL	100PROD4	100DSTL	150DSTL
100PROD5	100DSTL	150DSTL	100PROD6	100DSTL	150DSTL
150FEED1	100SPLT	150DSTL	Z100TOPS	100SPLT	----
150PROD1	150DSTL	150SPLT	150PROD2	150DSTL	200DSTL
150PROD3	150DSTL	200DSTL	150PROD4	150DSTL	200DSTL
150PROD5	150DSTL	200DSTL	150PROD6	150DSTL	200DSTL
200FEED1	150SPLT	200DSTL	Z150TOPS	150SPLT	----
200PROD1	200DSTL	200SPLT	200PROD2	200DSTL	----
250FEED1	200SPLT	----	Z200TOPS	200SPLT	----

FLWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
0ADSTL	0AFEED1 0AFEED2 0AFEED3	0APROD1 0APROD2 0APROD3
	0AFEED4 0AFEED5 0AFEED6	0APROD4 0APROD5 0APROD6
0BDSTL	0APROD1 0APROD2 0APROD3	0BPROD1 0BPROD2 0BPROD3
	0APROD4 0APROD5 0APROD6	0BPROD4 0BPROD5 0BPROD6
0CDSTL	0BPROD1 0BPROD2 0BPROD3	0CPROD1 0CPROD2 0CPROD3
	0BPROD4 0BPROD5 0BPROD6	0CPROD4 0CPROD5 0CPROD6
0DDSTL	0CPROD1 0CPROD2 0CPROD3	0DPROD1 0DPROD2 0DPROD3
	0CPROD4 0CPROD5 0CPROD6	0DPROD4 0DPROD5 0DPROD6
0EDSTL	0DPROD1 0DPROD2 0DPROD3	0EPROD1 0EPROD2 0EPROD3
	0DPROD4 0DPROD5 0DPROD6	0EPROD4 0EPROD5 0EPROD6
0FDSTL	0EPROD1 0EPROD2 0EPROD3	0FPROD1 0FPROD2 0FPROD3
	0EPROD4 0EPROD5 0EPROD6	0FPROD4 0FPROD5 0FPROD6
000DSTL	0FPROD1 0FPROD2 0FPROD3	000PROD1 000PROD2 000PROD3
	0FPROD4 0FPROD5 0FPROD6	000PROD4 000PROD5 000PROD6
050DSTL	000PROD1 000PROD2 000PROD3	050PROD1 050PROD2 050PROD3
	000PROD4 000PROD5 000PROD6	050PROD4 050PROD5 050PROD6
050SPLT	050PROD1	100FEED1 Z050TOPS
100DSTL	100FEED1 050PROD2 050PROD3	100PROD1 100PROD2 100PROD3
	050PROD4 050PROD5 050PROD6	100PROD4 100PROD5 100PROD6
100SPLT	100PROD1	150FEED1 Z100TOPS
150DSTL	150FEED1 100PROD2 100PROD3	150PROD1 150PROD2 150PROD3
	100PROD4 100PROD5 100PROD6	150PROD4 150PROD5 150PROD6

150SPLT	150PROD1	200FEED1	2150TOPS
200DSTL	200FEED1	150PROD2	150PROD3
	150PROD4	150PROD5	150PROD6
200SPLT	200PROD1	250FEED1	2200TOPS

COMPUTATION ORDER FOR THE FLOWSHEET IS:

OADSTL OBDSTL OCDSTL ODDSTL OEDSTL OFDSTL OOODSTL O5ODSTL O5OSPLT 100DSTL
100SPLT 150DSTL 150SPLT 200DSTL 200SPLT

MODULE apmod IS USED; CREATION DATE 07/31/91 10:15:30:25
LOCATED IN:E:\AP84A\xeq\apmod

NO ERRORS OR WARNINGS GENERATED
SIMULATION PROGRAM MAY BE EXECUTED

* ASPEN PLUS INPUT TRANSLATOR ENDS EXECUTION *

*** CALCULATION TRACE ***

D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75

SIMULATION CALCULATIONS BEGIN

ENTHALPY CALCULATION FOR INLET STREAM OAFEED1 OF BLOCK OADSTL
KODE = 3 NTRIAL = 4 T = 360.6 P = 0.1013E+06 V = 0.0000E+00

ENTHALPY CALCULATION FOR INLET STREAM OAFEED2 OF BLOCK OADSTL
KODE = 3 NTRIAL = 4 T = 360.6 P = 0.1013E+06 V = 0.0000E+00

ENTHALPY CALCULATION FOR INLET STREAM OAFEED3 OF BLOCK OADSTL
KODE = 3 NTRIAL = 4 T = 360.6 P = 0.1013E+06 V = 0.0000E+00

ENTHALPY CALCULATION FOR INLET STREAM OAFEED4 OF BLOCK OADSTL
KODE = 3 NTRIAL = 4 T = 360.6 P = 0.1013E+06 V = 0.0000E+00

ENTHALPY CALCULATION FOR INLET STREAM OAFEED5 OF BLOCK OADSTL
KODE = 3 NTRIAL = 4 T = 360.6 P = 0.1013E+06 V = 0.0000E+00

ENTHALPY CALCULATION FOR INLET STREAM OAFEED6 OF BLOCK OADSTL
KODE = 3 NTRIAL = 4 T = 360.6 P = 0.1013E+06 V = 0.0000E+00

UOS BLOCK OADSTL MODEL: RADFRAC

*** ITERATION HISTORY ***

*** OUTSIDE LOOP *** 1 1 2 0.93195E-03

*** OUTSIDE LOOP *** 2 1 2 0.53683E-04

UOS BLOCK OBDSTL MODEL: RADFRAC

*** ITERATION HISTORY ***

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*** OUTSIDE LOOP ***      1      1      2  0.12560E-02
*** OUTSIDE LOOP ***      2      1      2  0.63955E-04
      UOS BLOCK OCDSTL  MODEL: RADFRAC
*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***      1      1      2  0.14608E-02
*** OUTSIDE LOOP ***      2      1      2  0.65806E-04
      UOS BLOCK ODDSTL  MODEL: RADFRAC
*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***      1      1      2  0.15776E-02
*** OUTSIDE LOOP ***      2      1      2  0.64116E-04
      UOS BLOCK OEDSTL  MODEL: RADFRAC
*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***      1      1      2  0.16466E-02
*** OUTSIDE LOOP ***      2      1      2  0.61797E-04
      UOS BLOCK OFDSTL  MODEL: RADFRAC
*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***      1      1      2  0.16894E-02
*** OUTSIDE LOOP ***      2      1      2  0.59869E-04
      UOS BLOCK OOODSTL MODEL: RADFRAC
*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***      1      1      2  0.17165E-02
*** OUTSIDE LOOP ***      2      1      2  0.58493E-04
      UOS BLOCK O50DSTL MODEL: RADFRAC
*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***      1      1      2  0.25559E-02
*** OUTSIDE LOOP ***      2      1      2  0.30223E-03
*** OUTSIDE LOOP ***      3      1      1  0.25066E-04

```



```

UOS BLOCK 050SPLT  MODEL: FSPLIT
SPLIT FRACTIONS:  0.47619D-01    0.95238D+00

UOS BLOCK 100DSTL  MODEL: RADFRAC

*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***    1    1    2  0.41969E-02
*** OUTSIDE LOOP ***    2    1    2  0.46226E-03
*** OUTSIDE LOOP ***    3    1    2  0.58509E-04

UOS BLOCK 100SPLT  MODEL: FSPLIT
SPLIT FRACTIONS:  0.47619D-01    0.95238D+00

UOS BLOCK 150DSTL  MODEL: RADFRAC

*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***    1    1    2  0.17487E-02
*** OUTSIDE LOOP ***    2    1    2  0.11746E-03
*** OUTSIDE LOOP ***    3    1    1  0.11023E-04

UOS BLOCK 150SPLT  MODEL: FSPLIT
SPLIT FRACTIONS:  0.47619D-01    0.95238D+00

UOS BLOCK 200DSTL  MODEL: RADFRAC

*** ITERATION HISTORY ***

*** OUTSIDE LOOP ***    1    1    1  0.14718E-03
*** OUTSIDE LOOP ***    2    1    1  0.20913E-05

UOS BLOCK 200SPLT  MODEL: FSPLIT
SPLIT FRACTIONS:  0.00000D+00    0.10000D+01

SIMULATION CALCULATIONS COMPLETED

PDF UPDATED

REPORT WRITER ENTERED

REPORT GENERATED

NO ERRORS OR WARNINGS GENERATED

*****
* ASPEN PLUS SIMULATION PROGRAM ENDS EXECUTION *
*****

```

AAAAA	SSSSS	PPPPP	EEEE	NN	N	PPPPP	L	U	U	SSSSS	TM
A A	S	P P	E	N N	N	P P	L	U	U	S	
AAAAA	SSSSS	PPPPP	EEEE	N	N N	PPPPP	L	U	U	SSSSS	
A A	S	P	E	N	NN	P	L	U	U	S	
A A	SSSSS	P	EEEE	N	N	P	LLLLL	UUUUU		SSSSS	

HOTLINE:
U.S.A. 617-497-9010
EUROPE 31-70-3541051

**JANUARY 4, 1993
MONDAY
8:34:35 A.M.**

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0FPROD5 0FPROD6 000PROD1 000PROD2.....	48
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ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 1
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS VERSION OF ASPEN PLUS LICENSED TO SAN JOSE STATE UNIVERSITY
TYPE OF RUN: NEW

INPUT FILE NAME: 50D3RHUR.inp

OUTPUT PROBLEM DATA FILE NAME: 50D3RHUR VERSION NO. 1
LOCATED IN: E:\CHE_STOK\CHEXANE\HOLDUP\50D3RHUR

PDF SIZE USED FOR INPUT TRANSLATION:
NUMBER OF FILE RECORDS (PSIZE) = 99999
NUMBER OF IN-CORE RECORDS = 2000
PSIZE NEEDED FOR SIMULATION = 2000

CALLING PROGRAM NAME: apmod
LOCATED IN: E:\AP84A\xeq\apmod

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

BLOCK STATUS

```
*****
*
* ALL UNIT OPERATION BLOCKS WERE COMPLETED NORMALLY
*
*****
```

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
0AFEED6	----	0ADSTL	0AFEED5	----	0ADSTL
0AFEED4	----	0ADSTL	0AFEED3	----	0ADSTL
0AFEED2	----	0ADSTL	0AFEED1	----	0ADSTL
0APROD1	0ADSTL	0BDSTL	0APROD2	0ADSTL	0BDSTL
0APROD3	0ADSTL	0BDSTL	0APROD4	0ADSTL	0BDSTL
0APROD5	0ADSTL	0BDSTL	0APROD6	0ADSTL	0BDSTL
0BPROD1	0BDSTL	0CDSTL	0BPROD2	0BDSTL	0CDSTL
0BPROD3	0BDSTL	0CDSTL	0BPROD4	0BDSTL	0CDSTL
0BPROD5	0BDSTL	0CDSTL	0BPROD6	0BDSTL	0CDSTL
0CPROD1	0CDSTL	0DDSTL	0CPROD2	0CDSTL	0DDSTL
0CPROD3	0CDSTL	0DDSTL	0CPROD4	0CDSTL	0DDSTL
0CPROD5	0CDSTL	0DDSTL	0CPROD6	0CDSTL	0DDSTL
0DPROD1	0DDSTL	0EDSTL	0DPROD2	0DDSTL	0EDSTL
0DPROD3	0DDSTL	0EDSTL	0DPROD4	0DDSTL	0EDSTL
0DPROD5	0DDSTL	0EDSTL	0DPROD6	0DDSTL	0EDSTL
0EPROD1	0EDSTL	0FDSTL	0EPROD2	0EDSTL	0FDSTL
0EPROD3	0EDSTL	0FDSTL	0EPROD4	0EDSTL	0FDSTL
0EPROD5	0EDSTL	0FDSTL	0EPROD6	0EDSTL	0FDSTL
0FPROD1	0FDSTL	000DSTL	0FPROD2	0FDSTL	000DSTL
0FPROD3	0FDSTL	000DSTL	0FPROD4	0FDSTL	000DSTL
0FPROD5	0FDSTL	000DSTL	0FPROD6	0FDSTL	000DSTL
000PROD1	000DSTL	050DSTL	000PROD2	000DSTL	050DSTL
000PROD3	000DSTL	050DSTL	000PROD4	000DSTL	050DSTL
000PROD5	000DSTL	050DSTL	000PROD6	000DSTL	050DSTL
050PROD1	050DSTL	050SPLT	050PROD2	050DSTL	100DSTL
050PROD3	050DSTL	100DSTL	050PROD4	050DSTL	100DSTL
050PROD5	050DSTL	100DSTL	050PROD6	050DSTL	100DSTL
100FEED1	050SPLT	100DSTL	Z050TOPS	050SPLT	----
100PROD1	100DSTL	100SPLT	100PROD2	100DSTL	150DSTL
100PROD3	100DSTL	150DSTL	100PROD4	100DSTL	150DSTL
100PROD5	100DSTL	150DSTL	100PROD6	100DSTL	150DSTL
150FEED1	100SPLT	150DSTL	Z100TOPS	100SPLT	----
150PROD1	150DSTL	150SPLT	150PROD2	150DSTL	200DSTL
150PROD3	150DSTL	200DSTL	150PROD4	150DSTL	200DSTL
150PROD5	150DSTL	200DSTL	150PROD6	150DSTL	200DSTL
200FEED1	150SPLT	200DSTL	Z150TOPS	150SPLT	----
200PROD1	200DSTL	200SPLT	200PROD6	200DSTL	----
250FEED1	200SPLT	----	Z200TOPS	200SPLT	----

FLOWSHEET CONNECTIVITY BY BLOCKS

BLOCK	INLETS	OUTLETS
0ADSTL	0AFEED1 0AFEED2 0AFEED3 0AFEED4 0AFEED5 0AFEED6	0APROD1 0APROD2 0APROD3 0APROD4 0APROD5 0APROD6
0BDSTL	0APROD1 0APROD2 0APROD3 0APROD4 0APROD5 0APROD6	0BPROD1 0BPROD2 0BPROD3 0BPROD4 0BPROD5 0BPROD6
0CDSTL	0BPROD1 0BPROD2 0BPROD3 0BPROD4 0BPROD5 0BPROD6	0CPROD1 0CPROD2 0CPROD3 0CPROD4 0CPROD5 0CPROD6
0DDSTL	0CPROD1 0CPROD2 0CPROD3 0CPROD4 0CPROD5 0CPROD6	0DPROD1 0DPROD2 0DPROD3 0DPROD4 0DPROD5 0DPROD6
0EDSTL	0DPROD1 0DPROD2 0DPROD3	0EPROD1 0EPROD2 0EPROD3

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 3
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY BLOCKS (CONTINUED)

	ODPROD4	ODPROD5	ODPROD6	OEPROD4	OEPROD5	OEPROD6
0FDSTL	OEPROD1	OEPROD2	OEPROD3	OFFPROD1	OFFPROD2	OFFPROD3
	OEPROD4	OEPROD5	OEPROD6	OFFPROD4	OFFPROD5	OFFPROD6
000DSTL	OFFPROD1	OFFPROD2	OFFPROD3	000PROD1	000PROD2	000PROD3
	OFFPROD4	OFFPROD5	OFFPROD6	000PROD4	000PROD5	000PROD6
050DSTL	000PROD1	000PROD2	000PROD3	050PROD1	050PROD2	050PROD3
	000PROD4	000PROD5	000PROD6	050PROD4	050PROD5	050PROD6
050SPLT	050PROD1			100FEED1	Z050TOPS	
100DSTL	100FEED1	050PROD2	050PROD3	100PROD1	100PROD2	100PROD3
	050PROD4	050PROD5	050PROD6	100PROD4	100PROD5	100PROD6
100SPLT	100PROD1			150FEED1	Z100TOPS	
150DSTL	150FEED1	100PROD2	100PROD3	150PROD1	150PROD2	150PROD3
	100PROD4	100PROD5	100PROD6	150PROD4	150PROD5	150PROD6
150SPLT	150PROD1			200FEED1	Z150TOPS	
200DSTL	200FEED1	150PROD2	150PROD3	200PROD1	200PROD6	
	150PROD4	150PROD5	150PROD6			
200SPLT	200PROD1			250FEED1	Z200TOPS	

COMPUTATIONAL SEQUENCE

SEQUENCE USED WAS:

OADSTL OBDSTL OCDSTL ODDSTL OEDSTL OFDSTL 000DSTL 050DSTL 050SPLT
100DSTL 100SPLT 150DSTL 150SPLT 200DSTL 200SPLT

OVERALL FLOWSHEET BALANCE

	*** MASS AND ENERGY BALANCE ***		
CONVENTIONAL COMPONENTS (KMOL/HR)	IN	OUT	RELATIVE DIFF.
C6H12	0.124062	0.124062	-0.251883E-10
C7H8	0.760380E-01	0.760380E-01	-0.365799E-08
TOTAL BALANCE			
MOLE (KMOL/HR)	0.200100	0.200100	-0.140565E-08
MASS (KG/HR)	17.4475	17.4475	-0.148397E-08
ENTHALPY (CAL/SEC)	-1081.71	-1078.70	-0.278363E-02

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 4
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
PHYSICAL PROPERTIES SECTION

COMPONENTS

ID	TYPE	FORMULA	NAME OR ALIAS	REPORT NAME
C6H12	C	C6H12-1	CYCLOHEXANE	C6H12
C7H8	C	C7H8	TOLUENE	C7H8

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 5
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CV=0.75
U-O-S BLOCK SECTION

BLOCK: OADSTL MODEL: RADFRAC

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-----
INLETS  - OAFEED1 STAGE 1
          OAFEED2 STAGE 2
          OAFEED3 STAGE 3
          OAFEED4 STAGE 4
          OAFEED5 STAGE 5
          OAFEED6 STAGE 6
OUTLETS  - OAPROD1 STAGE 1
          OAPROD2 STAGE 2
          OAPROD3 STAGE 3
          OAPROD4 STAGE 4
          OAPROD5 STAGE 5
          OAPROD6 STAGE 6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	0.180321E-13
MASS(KG/HR)	17.4475	17.4475	0.169007E-13
ENTHALPY(CAL/SEC)	-1081.71	-1081.70	-0.891931E-05

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 6
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OADSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000

**** PROFILES ****

P-SPEC	STAGE	1	PRES, ATM	1.00000
--------	-------	---	-----------	---------

**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	1.0000
	2		0.75000
	3		0.75000
	4		0.75000
	5		0.75000
	6		1.0000

**** RESULTS ****

TOP STAGE TEMPERATURE	K	357.337
BOTTOM STAGE TEMPERATURE	K	360.761
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0074072
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.039484
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.2955
REBOILER DUTY	CAL/SEC	15.3029

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.63391E-05	STAGE=	1
BUBBLE POINT	0.16820E-04	STAGE=	1
COMPONENT MASS BALANCE	0.29400E-12	STAGE=	3 COMP=C7H8
ENERGY BALANCE	0.58214E-04	STAGE=	1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 7
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OADSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	357.34	1.0000	-26444.	-23086.	-15.2955
2	358.41	1.0000	-24045.	-21430.	
3	359.17	1.0000	-22411.	-20544.	
4	359.73	1.0000	-21267.	-19890.	
5	360.16	1.0000	-20397.	-19349.	
6	360.76	1.0000	-19231.	-18789.	15.3029

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		MIXED	PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR			LIQUID	VAPOR
1	0.7500E-02	0.0000E+00				.25000-02	.25000-02	
2	0.7469E-02	0.7500E-02				.25000-02	.25000-02	
3	0.7446E-02	0.7469E-02				.25000-02	.25000-02	
4	0.7429E-02	0.7446E-02				.25000-02	.25000-02	
5	0.7407E-02	0.7429E-02				.25000-02	.25000-02	
6	0.1876	0.7407E-02				0.1876	0.1876	

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.78996	.21004
2	.73154	.26846
3	.69176	.30824
4	.66393	.33607
5	.64277	.35723
6	.61440	.38560

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.88587	.11413
2	.84661	.15339
3	.82576	.17424
4	.81036	.18964
5	.79759	.20241
6	.78451	.21549

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.1215	.54327
2	1.1668	.54543
3	1.2012	.54858
4	1.2269	.55164
5	1.2476	.55443
6	1.2768	.55887

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 8
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OBDSTL MODEL: RADFRAC

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INLETS  - OAPROD1 STAGE 1
          OAPROD2 STAGE 2
          OAPROD3 STAGE 3
          OAPROD4 STAGE 4
          OAPROD5 STAGE 5
          OAPROD6 STAGE 6
OUTLETS  - OBPROD1 STAGE 1
          OBPROD2 STAGE 2
          OBPROD3 STAGE 3
          OBPROD4 STAGE 4
          OBPROD5 STAGE 5
          OBPROD6 STAGE 6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	0.484093E-13
MASS(KG/HR)	17.4475	17.4475	0.460188E-13
ENTHALPY(CAL/SEC)	-1081.70	-1081.68	-0.123592E-04

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 9
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OBDSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE	1	PRES, ATM	1.00000
--------	-------	---	-----------	---------

**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	1.0000
	2		0.75000
	3		0.75000
	4		0.75000
	5		0.75000
	6		1.0000

**** RESULTS ****

TOP STAGE TEMPERATURE	K	356.063
BOTTOM STAGE TEMPERATURE	K	360.850
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0073475
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.039166
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.1748
REBOILER DUTY	CAL/SEC	15.1857

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.35867E-05	STAGE=	5
BUBBLE POINT	0.14053E-04	STAGE=	5
COMPONENT MASS BALANCE	0.10159E-11	STAGE=	3 COMP=C7H8
ENERGY BALANCE	0.49621E-04	STAGE=	1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 10
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OBDSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	356.06	1.0000	-29480.	-24778.	-15.1747
2	356.97	1.0000	-27306.	-23208.	
3	357.84	1.0000	-25302.	-22096.	
4	358.66	1.0000	-23488.	-21041.	
5	359.48	1.0000	-21766.	-19958.	
6	360.85	1.0000	-19060.	-18679.	15.1857

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR	MIXED	LIQUID	VAPOR
1	0.7500E-02	0.0000E+00				.25000-02	.25000-02
2	0.7465E-02	0.7500E-02				.25000-02	.25000-02
3	0.7431E-02	0.7465E-02				.25000-02	.25000-02
4	0.7398E-02	0.7431E-02				.25000-02	.25000-02
5	0.7347E-02	0.7398E-02				.25000-02	.25000-02
6	0.1876	0.7347E-02				0.1876	0.1876

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.86389	.13611
2	.81095	.18905
3	.76213	.23787
4	.71797	.28203
5	.67607	.32393
6	.61026	.38974

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.92584	.74159E-01
2	.88854	.11146
3	.86230	.13770
4	.83739	.16261
5	.81182	.18818
6	.78191	.21809

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.0717	.54474
2	1.1065	.54322
3	1.1424	.54393
4	1.1782	.54634
5	1.2155	.55021
6	1.2813	.55958

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 11
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OCDSTL MODEL: RADFRAC

```

INLETS  - OBPROD1 STAGE 1
          OBPROD2 STAGE 2
          OBPROD3 STAGE 3
          OBPROD4 STAGE 4
          OBPROD5 STAGE 5
          OBPROD6 STAGE 6
OUTLETS - OCPROD1 STAGE 1
          OCPROD2 STAGE 2
          OCPROD3 STAGE 3
          OCPROD4 STAGE 4
          OCPROD5 STAGE 5
          OCPROD6 STAGE 6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	0.853057E-13
MASS(KG/HR)	17.4475	17.4475	0.808383E-13
ENTHALPY(CAL/SEC)	-1081.68	-1081.67	-0.992017E-05

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 12
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: .OCDSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000

**** PROFILES ****

P-SPEC	STAGE 1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	1.0000
	2		0.75000
	3		0.75000
	4		0.75000
	5		0.75000
	6		1.0000

**** RESULTS ****

TOP STAGE TEMPERATURE	K	355.434
BOTTOM STAGE TEMPERATURE	K	360.912
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0073119
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.038976
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.1061
REBOILER DUTY	CAL/SEC	15.1144

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.36193E-05	STAGE=	5
BUBBLE POINT	0.14021E-04	STAGE=	5
COMPONENT MASS BALANCE	0.17721E-11	STAGE=	3 COMP=C7H8
ENERGY BALANCE	0.39478E-04	STAGE=	1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 13
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OCDSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	355.43	1.0000	-31050.	-25648.	-15.1060
2	356.13	1.0000	-29305.	-24321.	
3	356.93	1.0000	-27395.	-23217.	
4	357.82	1.0000	-25335.	-21981.	
5	358.87	1.0000	-23038.	-20514.	
6	360.91	1.0000	-18943.	-18603.	15.1143

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR VAPOR	MIXED	PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR				LIQUID	VAPOR
1	0.7500E-02	0.0000E+00			.25000-02	.25000-02	
2	0.7467E-02	0.7500E-02			.25000-02	.25000-02	
3	0.7431E-02	0.7467E-02			.25000-02	.25000-02	
4	0.7388E-02	0.7431E-02			.25000-02	.25000-02	
5	0.7312E-02	0.7388E-02			.25000-02	.25000-02	
6	0.1876	0.7312E-02			0.1876	0.1876	

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.90210	.97895E-01
2	.85963	.14037
3	.81311	.18689
4	.76293	.23707
5	.70702	.29298
6	.60741	.39259

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.94641	.53593E-01
2	.91484	.85158E-01
3	.88872	.11128
4	.85950	.14050
5	.82481	.17519
6	.78012	.21988

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.0491	.54735
2	1.0744	.54453
3	1.1050	.54323
4	1.1417	.54390
5	1.1876	.54719
6	1.2843	.56008

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 14
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: ODDSTL MODEL: RADFRAC

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INLETS  -  OCPROD1  STAGE  1
           OCPROD2  STAGE  2
           OCPROD3  STAGE  3
           OCPROD4  STAGE  4
           OCPROD5  STAGE  5
           OCPROD6  STAGE  6
OUTLETS  -  ODPROD1  STAGE  1
           ODPROD2  STAGE  2
           ODPROD3  STAGE  3
           ODPROD4  STAGE  4
           ODPROD5  STAGE  5
           ODPROD6  STAGE  6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	0.200100	0.200100	0.109857E-12
MASS (KG/HR)	17.4475	17.4475	0.104051E-12
ENTHALPY (CAL/SEC)	-1081.67	-1081.67	-0.692060E-05

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 15
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: ODDSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE 1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	
	2	1.0000	
	3	0.75000	
	4	0.75000	
	5	0.75000	
	6	0.75000	
		1.0000	

**** RESULTS ****

TOP STAGE TEMPERATURE	K	355.085
BOTTOM STAGE TEMPERATURE	K	360.953
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0072907
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.038863
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.0656
REBOILER DUTY	CAL/SEC	15.0707

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.32959E-05	STAGE= 5
BUBBLE POINT	0.12285E-04	STAGE= 5
COMPONENT MASS BALANCE	0.23488E-11	STAGE= 4 COMP=C7H8
ENERGY BALANCE	0.31969E-04	STAGE= 1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 16
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF/CY=0.75
U-O-S BLOCK SECTION

BLOCK: ODDSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	355.08	1.0000	-31942.	-26144.	-15.0656
2	355.65	1.0000	-30515.	-25008.	
3	356.35	1.0000	-28772.	-23958.	
4	357.25	1.0000	-26653.	-22646.	
5	358.42	1.0000	-24013.	-20933.	
6	360.95	1.0000	-18866.	-18553.	15.0706

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR	MIXED	LIQUID	VAPOR
1	0.7500E-02	0.0000E+00				.25000-02	.25000-02
2	0.7471E-02	0.7500E-02				.25000-02	.25000-02
3	0.7433E-02	0.7471E-02				.25000-02	.25000-02
4	0.7385E-02	0.7433E-02				.25000-02	.25000-02
5	0.7291E-02	0.7385E-02				.25000-02	.25000-02
6	0.1876	0.7291E-02				0.1876	0.1876

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.92385	.76152E-01
2	.88908	.11092
3	.84665	.15335
4	.79504	.20496
5	.73074	.26926
6	.60554	.39446

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.95815	.41846E-01
2	.93110	.68904E-01
3	.90621	.93789E-01
4	.87514	.12486
5	.83460	.16540
6	.77894	.22106

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.0371	.54940
2	1.0566	.54632
3	1.0826	.54398
4	1.1178	.54322
5	1.1675	.54546
6	1.2864	.56042

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 17
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OEDSTL MODEL: RADFRAC

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INLETS  -  ODPROD1  STAGE  1
          ODPROD2  STAGE  2
          ODPROD3  STAGE  3
          ODPROD4  STAGE  4
          ODPROD5  STAGE  5
          ODPROD6  STAGE  6
OUTLETS  -  OEPROD1  STAGE  1
          OEPROD2  STAGE  2
          OEPROD3  STAGE  3
          OEPROD4  STAGE  4
          OEPROD5  STAGE  5
          OEPROD6  STAGE  6

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PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	0.122064E-12
MASS(KG/HR)	17.4475	17.4475	0.116472E-12
ENTHALPY(CAL/SEC)	-1081.67	-1081.66	-0.456611E-05

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 18
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 0EDSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE 1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	
	2		1.0000
	3		0.75000
	4		0.75000
	5		0.75000
	6		0.75000
			1.0000

**** RESULTS ****

TOP STAGE TEMPERATURE	K	354.878
BOTTOM STAGE TEMPERATURE	K	360.979
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0072778
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.038794
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.0413
REBOILER DUTY	CAL/SEC	15.0438

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.29333E-05	STAGE= 5
BUBBLE POINT	0.10516E-04	STAGE= 5
COMPONENT MASS BALANCE	0.29298E-11	STAGE= 4 COMP=C7H8
ENERGY BALANCE	0.27036E-04	STAGE= 1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 19
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OEDSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	354.88	1.0000	-32476.	-26442.	-15.0413
2	355.35	1.0000	-31253.	-25433.	
3	356.00	1.0000	-29647.	-24431.	
4	356.87	1.0000	-27530.	-23086.	
5	358.11	1.0000	-24690.	-21221.	
6	360.98	1.0000	-18817.	-18521.	15.0437

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR	MIXED	LIQUID	VAPOR
1	0.7500E-02	0.0000E+00				.25000-02	.25000-02
2	0.7473E-02	0.7500E-02				.25000-02	.25000-02
3	0.7436E-02	0.7473E-02				.25000-02	.25000-02
4	0.7385E-02	0.7436E-02				.25000-02	.25000-02
5	0.7278E-02	0.7385E-02				.25000-02	.25000-02
6	0.1876	0.7278E-02				0.1876	0.1876

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.93683	.63171E-01
2	.90705	.92952E-01
3	.86795	.13205
4	.81640	.18360
5	.74723	.25277
6	.60434	.39566

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.96520	.34803E-01
2	.94116	.58844E-01
3	.91740	.82598E-01
4	.88552	.11448
5	.84132	.15868
6	.77818	.22182

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.0303	.55083
2	1.0464	.54778
3	1.0692	.54496
4	1.1027	.54326
5	1.1541	.54454
6	1.2877	.56063

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 20
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OFDSTL MODEL: RADFRAC

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INLETS  - OEPROD1 STAGE 1
          OEPROD2 STAGE 2
          OEPROD3 STAGE 3
          OEPROD4 STAGE 4
          OEPROD5 STAGE 5
          OEPROD6 STAGE 6
OUTLETS - OFPROD1 STAGE 1
          OFPROD2 STAGE 2
          OFPROD3 STAGE 3
          OFPROD4 STAGE 4
          OFPROD5 STAGE 5
          OFPROD6 STAGE 6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	0.127473E-12
MASS(KG/HR)	17.4475	17.4475	0.121156E-12
ENTHALPY(CAL/SEC)	-1081.66	-1081.66	-0.289564E-05

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 21
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OFDSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000

**** PROFILES ****

P-SPEC	STAGE	1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	1.0000
	2		0.75000
	3		0.75000
	4		0.75000
	5		0.75000
	6		1.0000

**** RESULTS ****

TOP STAGE TEMPERATURE	K	354.753
BOTTOM STAGE TEMPERATURE	K	360.995
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0072700
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.038752
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.0264
REBOILER DUTY	CAL/SEC	15.0271

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.26476E-05	STAGE=	5
BUBBLE POINT	0.91914E-05	STAGE=	5
COMPONENT MASS BALANCE	0.32498E-11	STAGE=	4 COMP=C7H8
ENERGY BALANCE	0.23903E-04	STAGE=	1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 22
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: OFDSTL MODEL: RADFRAC (CONTINUED)

***** PROFILES *****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	354.75	1.0000	-32801.	-26624.	-15.0264
2	355.18	1.0000	-31707.	-25697.	
3	355.77	1.0000	-30196.	-24730.	
4	356.63	1.0000	-28094.	-23369.	
5	357.91	1.0000	-25137.	-21409.	
6	361.00	1.0000	-18785.	-18501.	15.0271

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR	MIXED	LIQUID	VAPOR
1	0.7500E-02	0.0000E+00				.25000-02	.25000-02
2	0.7475E-02	0.7500E-02				.25000-02	.25000-02
3	0.7438E-02	0.7475E-02				.25000-02	.25000-02
4	0.7385E-02	0.7438E-02				.25000-02	.25000-02
5	0.7270E-02	0.7385E-02				.25000-02	.25000-02
6	0.1876	0.7270E-02				0.1876	0.1876

***** X-PROFILE *****

STAGE	C6H12	C7H8
1	.94476	.55243E-01
2	.91811	.81893E-01
3	.88132	.11868
4	.83013	.16987
5	.75811	.24189
6	.60358	.39642

***** Y-PROFILE *****

STAGE	C6H12	C7H8
1	.96951	.30487E-01
2	.94740	.52600E-01
3	.92446	.75542E-01
4	.89219	.10781
5	.84573	.15427
6	.77770	.22230

***** K-VALUES *****

STAGE	C6H12	C7H8
1	1.0262	.55178
2	1.0403	.54882
3	1.0612	.54577
4	1.0934	.54349
5	1.1455	.54407
6	1.2885	.56077

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 23
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 000DSTL MODEL: RADFRAC

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-----
INLETS  - OFPROD1 STAGE 1
          OFPROD2 STAGE 2
          OFPROD3 STAGE 3
          OFPROD4 STAGE 4
          OFPROD5 STAGE 5
          OFPROD6 STAGE 6
OUTLETS  - 000PROD1 STAGE 1
          000PROD2 STAGE 2
          000PROD3 STAGE 3
          000PROD4 STAGE 4
          000PROD5 STAGE 5
          000PROD6 STAGE 6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	0.129692E-12
MASS(KG/HR)	17.4475	17.4475	0.123395E-12
ENTHALPY(CAL/SEC)	-1081.66	-1081.66	-0.182147E-05

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 24
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 000DSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.0025000
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE 1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY
2	1.0000	
3	0.75000	
4	0.75000	
5	0.75000	
6	0.75000	
	1.0000	

**** RESULTS ****

TOP STAGE TEMPERATURE	K	354.676
BOTTOM STAGE TEMPERATURE	K	361.006
TOP STAGE LIQUID FLOW	KMOL/HR	0.0075000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.18760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.0072651
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		0.038727
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-15.0173
REBOILER DUTY	CAL/SEC	15.0168

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.24492E-05	STAGE= 5
BUBBLE POINT	0.83005E-05	STAGE= 5
COMPONENT MASS BALANCE	0.34142E-11	STAGE= 4 COMP=C7H8
ENERGY BALANCE	0.23464E-04	STAGE= 5

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 25
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 000DSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	354.68	1.0000	-33002.	-26737.	-15.0172
2	355.07	1.0000	-31988.	-25861.	
3	355.64	1.0000	-30538.	-24917.	
4	356.49	1.0000	-28451.	-23548.	
5	357.78	1.0000	-25424.	-21530.	
6	361.01	1.0000	-18766.	-18488.	15.0167

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		MIXED	PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR			LIQUID	VAPOR
1	0.7500E-02	0.0000E+00				.25000-02	.25000-02	
2	0.7476E-02	0.7500E-02				.25000-02	.25000-02	
3	0.7440E-02	0.7476E-02				.25000-02	.25000-02	
4	0.7385E-02	0.7440E-02				.25000-02	.25000-02	
5	0.7265E-02	0.7385E-02				.25000-02	.25000-02	
6	0.1876	0.7265E-02				.25000-02	.25000-02	
						0.1876	0.1876	

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.94965	.50348E-01
2	.92495	.75048E-01
3	.88966	.11034
4	.83882	.16118
5	.76510	.23490
6	.60310	.39690

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.97218	.27816E-01
2	.95128	.48716E-01
3	.92888	.71122E-01
4	.89640	.10360
5	.84855	.15145
6	.77740	.22260

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.0237	.55240
2	1.0366	.54952
3	1.0563	.54636
4	1.0877	.54372
5	1.1400	.54382
6	1.2890	.56085

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 26
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 050DSTL MODEL: RADFRAC

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INLETS  - 000PROD1 STAGE 1
          000PROD2 STAGE 2
          000PROD3 STAGE 3
          000PROD4 STAGE 4
          000PROD5 STAGE 5
          000PROD6 STAGE 6
OUTLETS - 050PROD1 STAGE 1
          050PROD2 STAGE 2
          050PROD3 STAGE 3
          050PROD4 STAGE 4
          050PROD5 STAGE 5
          050PROD6 STAGE 6

```

PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.200100	0.200100	-0.127038E-08
MASS(KG/HR)	17.4475	17.4475	-0.134583E-08
ENTHALPY(CAL/SEC)	-1081.66	-1081.19	-0.434399E-03

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 27
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 050DSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.052500
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE	1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	1.0000
	2		0.75000
	3		0.75000
	4		0.75000
	5		0.75000
	6		1.0000

**** RESULTS ****

TOP STAGE TEMPERATURE	K	355.174
BOTTOM STAGE TEMPERATURE	K	363.530
TOP STAGE LIQUID FLOW	KMOL/HR	0.15750
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.13760
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.19943
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		1.44938
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-417.557
REBOILER DUTY	CAL/SEC	418.028

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.12884E-05	STAGE=	5
BUBBLE POINT	0.10026E-04	STAGE=	4
COMPONENT MASS BALANCE	0.54069E-07	STAGE=	3 COMP=C7H8
ENERGY BALANCE	0.68799E-05	STAGE=	1

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 28
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 050DSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	355.17	1.0000	-31712.	-26016.	-417.5572
2	355.94	1.0000	-29789.	-24452.	
3	356.97	1.0000	-27304.	-22926.	
4	358.36	1.0000	-24136.	-20955.	
5	360.23	1.0000	-20255.	-18452.	
6	363.53	1.0000	-14344.	-15387.	418.0275

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID VAPOR
1	0.1575	0.0000E+00			.25000-02	.52500-01
2	0.1563	0.2075			.25000-02	.25000-02
3	0.1547	0.2063			.25000-02	.25000-02
4	0.1527	0.2047			.25000-02	.25000-02
5	0.1494	0.2027			.25000-02	.25000-02
6	0.1376	0.1994			0.1876	0.1376

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.91822	.81775E-01
2	.87140	.12860
3	.81088	.18912
4	.73376	.26624
5	.63931	.36069
6	.49576	.50424

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.95512	.44880E-01
2	.91785	.82154E-01
3	.88172	.11828
4	.83509	.16491
5	.77595	.22405
6	.70429	.29571

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.0402	.54883
2	1.0671	.54515
3	1.1065	.54321
4	1.1650	.54529
5	1.2511	.55495
6	1.4206	.58645

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 29
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 050SPLT MODEL: FSPLIT

INLET STREAM: 050PROD1
OUTLET STREAMS: 100FEED1 Z050TOPS
PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	0.525000E-01	0.525000E-01	0.000000E+00
MASS (KG/HR)	4.45276	4.45276	0.000000E+00
ENTHALPY (CAL/SEC)	-462.460	-462.460	0.000000E+00

*** INPUT DATA ***

MOLE-FLOW (KMOL/HR) STRM=100FEED1 FLOW= 0.0025000 KEY= 0

*** RESULTS ***

STREAM= 100FEED1 SPLIT= 0.047619 KEY= 0
Z050TOPS 0.95238 0

BLOCK: 100DSTL MODEL: RADFRAC

INLETS - 100FEED1 STAGE 1
050PROD2 STAGE 2
050PROD3 STAGE 3
050PROD4 STAGE 4
050PROD5 STAGE 5
050PROD6 STAGE 6
OUTLETS - 100PROD1 STAGE 1
100PROD2 STAGE 2
100PROD3 STAGE 3
100PROD4 STAGE 4
100PROD5 STAGE 5
100PROD6 STAGE 6
PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***		
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	0.150100	0.150100	0.129440E-14
MASS (KG/HR)	13.2068	13.2068	0.134503E-14
ENTHALPY (CAL/SEC)	-640.748	-639.396	-0.210982E-02

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 30
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 100DSTL MODEL: RADFRAC (CONTINUED)

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.052500
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE 1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE 1	EFFICIENCY	1.0000
2		0.75000
3		0.75000
4		0.75000
5		0.75000
6		1.0000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 31
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 100DSTL MODEL: RADFRAC (CONTINUED)

**** RESULTS ****

TOP STAGE TEMPERATURE	K	356.136
BOTTOM STAGE TEMPERATURE	K	369.116
TOP STAGE LIQUID FLOW	KMOL/HR	0.15750
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.087600
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.19612
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		2.23878
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-421.341
REBOILER DUTY	CAL/SEC	422.671

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.68669E-04	STAGE=	6
BUBBLE POINT	0.34887E-04	STAGE=	6
COMPONENT MASS BALANCE	0.14701E-13	STAGE=	1 COMP=C7H8
ENERGY BALANCE	0.40259E-04	STAGE=	1

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	356.14	1.0000	-29300.	-24678.	-421.3408
2	357.54	1.0000	-25974.	-21961.	
3	359.46	1.0000	-21806.	-19321.	
4	362.00	1.0000	-16944.	-16025.	
5	365.08	1.0000	-11934.	-12203.	
6	369.12	1.0000	-6528.9	-8280.4	422.6705

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR	MIXED	LIQUID	VAPOR
1	0.1575	0.0000E+00				.25000-02	.52500-01
2	0.1553	0.2075				.25000-02	.25000-02
3	0.1526	0.2053				.25000-02	.25000-02
4	0.1496	0.2026				.25000-02	.25000-02
5	0.1461	0.1996				.25000-02	.25000-02
6	0.8760E-01	0.1961			0.1376		.87600-01

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 32
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 100DSTL MODEL: RADFRAC (CONTINUED)

STAGE	C6H12	C7H8	X-PROFILE
1	.85950	.14050	
2	.77849	.22151	
3	.67705	.32295	
4	.55886	.44114	
5	.43742	.56258	
6	.30705	.69295	

STAGE	C6H12	C7H8	Y-PROFILE
1	.92349	.76511E-01	
2	.85879	.14121	
3	.79637	.20363	
4	.71855	.28145	
5	.62841	.37159	
6	.53658	.46342	

STAGE	C6H12	C7H8	K-VALUES
1	1.0745	.54452	
2	1.1299	.54347	
3	1.2146	.55013	
4	1.3395	.56989	
5	1.5065	.60613	
6	1.7475	.66883	

BLOCK: 100SPLT MODEL: FSPLIT

INLET STREAM: 100PROD1
OUTLET STREAMS: 150FEED1 Z100TOPS
PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

	*** MASS AND ENERGY BALANCE ***	RELATIVE DIFF.
TOTAL BALANCE	IN OUT	
MOLE(KMOL/HR)	0.525000E-01 0.525000E-01	0.000000E+00
MASS(KG/HR)	4.47736 4.47736	0.000000E+00
ENTHALPY(CAL/SEC)	-427.291 -427.291	0.000000E+00

*** INPUT DATA ***

MOLE-FLOW (KMOL/HR) STRM=150FEED1 FLOW= 0.0025000 KEY= 0

*** RESULTS ***

STREAM= 150FEED1 SPLIT= 0.047619 KEY= 0
Z100TOPS 0.95238 0

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 33
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 150DSTL MODEL: RADFRAC

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INLETS  - 150FEED1 STAGE 1
          100PROD2 STAGE 2
          100PROD3 STAGE 3
          100PROD4 STAGE 4
          100PROD5 STAGE 5
          100PROD6 STAGE 6
OUTLETS  - 150PROD1 STAGE 1
          150PROD2 STAGE 2
          150PROD3 STAGE 3
          150PROD4 STAGE 4
          150PROD5 STAGE 5
          150PROD6 STAGE 6
PROPERTY OPTION SET:  SYSOP7  UNIFAC / REDLICH-KWONG

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*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	0.100100	0.100100	-0.271668E-09
MASS (KG/HR)	8.94265	8.94265	-0.270681E-09
ENTHALPY (CAL/SEC)	-232.452	-230.968	-0.638432E-02

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 34
 D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
 U-O-S BLOCK SECTION

BLOCK: 150DSTL MODEL: RADFRAC (CONTINUED)

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.052500
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE 1	PRES, ATM	1.00000
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**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY
2	1.0000	
3	0.75000	
4	0.75000	
5	0.75000	
6	1.0000	

 **** RESULTS ****

TOP STAGE TEMPERATURE	K	361.781
BOTTOM STAGE TEMPERATURE	K	378.854
TOP STAGE LIQUID FLOW	KMOL/HR	0.15750
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.037600
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.20005
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		5.32056
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-441.726
REBOILER DUTY	CAL/SEC	443.210

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.15230E-05	STAGE= 5
BUBBLE POINT	0.69052E-05	STAGE= 2
COMPONENT MASS BALANCE	0.10023E-07	STAGE= 1 COMP=C7H8
ENERGY BALANCE	0.11587E-04	STAGE= 5

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 35
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 150DSTL MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	361.78	1.0000	-17340.	-17537.	-441.7257
2	366.62	1.0000	-9724.1	-9531.8	
3	371.55	1.0000	-3768.7	-3426.5	
4	375.28	1.0000	-119.02	1341.7	
5	377.51	1.0000	1800.9	4308.4	
6	378.85	1.0000	2882.2	5925.9	443.2096

STAGE	FLOW RATE KMOL/HR		LIQUID	FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR		VAPOR	MIXED	LIQUID	VAPOR
1	0.1575	0.0000E+00				.25000-02	.52500-01
2	0.1532	0.2075				.25000-02	.25000-02
3	0.1510	0.2032				.25000-02	.25000-02
4	0.1503	0.2010				.25000-02	.25000-02
5	0.1501	0.2003				.25000-02	.25000-02
6	0.3760E-01	0.2001				.87600-01	.37600-01

**** X-PROFILE ****

STAGE	C6H12	C7H8
1	.56845	.43155
2	.38401	.61599
3	.24085	.75915
4	.15384	.84616
5	.10835	.89165
6	.82834E-01	.91717

**** Y-PROFILE ****

STAGE	C6H12	C7H8
1	.75499	.24501
2	.56495	.43505
3	.42095	.57905
4	.30839	.69161
5	.23828	.76172
6	.20015	.79985

**** K-VALUES ****

STAGE	C6H12	C7H8
1	1.3282	.56775
2	1.5961	.62836
3	1.9035	.71334
4	2.1565	.78973
5	2.3164	.84003
6	2.4163	.87209

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 36
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 150SPLIT MODEL: FSPLIT

INLET STREAM: 150PROD1
OUTLET STREAMS: 200FEED1 Z150TOPS
PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.525000E-01	0.525000E-01	0.000000E+00
MASS(KG/HR)	4.59928	4.59928	0.000000E+00
ENTHALPY(CAL/SEC)	-252.869	-252.869	0.000000E+00

*** INPUT DATA ***

MOLE-FLOW (KMOL/HR) STRM=200FEED1 FLOW= 0.0025000 KEY= 0

*** RESULTS ***

STREAM= 200FEED1 SPLIT= 0.047619 KEY= 0
Z150TOPS 0.95238 0

BLOCK: 200DSTL MODEL: RADFRAC

INLETS - 200FEED1 STAGE 1
150PROD2 STAGE 2
150PROD3 STAGE 3
150PROD4 STAGE 4
150PROD5 STAGE 5
150PROD6 STAGE 6
OUTLETS - 200PROD1 STAGE 1
200PROD6 STAGE 6
PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

*** MASS AND ENERGY BALANCE ***			
	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE(KMOL/HR)	0.501000E-01	0.501000E-01	-0.655109E-13
MASS(KG/HR)	4.56238	4.56238	-0.605437E-13
ENTHALPY(CAL/SEC)	9.85931	9.51332	0.350926E-01

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 37
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 200DSTL MODEL: RADFRAC (CONTINUED)

**** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	6
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	NEWTON
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	25
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	50
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MOLAR REFLUX RATIO	3.00000
MOLAR DISTILLATE RATE	0.050000
	KMOL/HR

**** PROFILES ****

P-SPEC	STAGE	1	PRES, ATM	1.00000
--------	-------	---	-----------	---------

**** TRAY MURPHREE EFFICIENCY ****

STAGE	1	EFFICIENCY	1.0000
	2		0.75000
	3		0.75000
	4		0.75000
	5		0.75000
	6		1.0000

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 38
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 200DSTL MODEL: RADFRAC (CONTINUED)

**** RESULTS ****

TOP STAGE TEMPERATURE	K	376.172
BOTTOM STAGE TEMPERATURE	K	383.206
TOP STAGE LIQUID FLOW	KMOL/HR	0.15000
BOTTOM STAGE LIQUID FLOW	KMOL/HR	0.00010000
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOTTOM STAGE VAPOR FLOW	KMOL/HR	0.19815
MOLAR REFLUX RATIO		3.00000
MOLAR BOILUP RATIO		1,981.47
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-437.833
REBOILER DUTY	CAL/SEC	437.487

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.79455E-06	STAGE=	1
BUBBLE POINT	0.12954E-05	STAGE=	1
COMPONENT MASS BALANCE	0.20510E-07	STAGE=	6 COMP=C6H12
ENERGY BALANCE	0.42127E-05	STAGE=	1

**** PROFILES ****

STAGE	TEMPERATURE K	PRESSURE ATM	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	376.17	1.0000	672.91	1725.0	-437.8333
2	380.15	1.0000	3866.8	8881.6	
3	381.96	1.0000	5175.3	11473.	
4	382.72	1.0000	5697.7	12587.	
5	383.04	1.0000	5913.2	13065.	
6	383.21	1.0000	6024.3	13286.	437.4869

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR		PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	LIQUID	VAPOR
1	0.1500	0.0000E+00			.25000-02	.50000-01
2	0.1527	0.1975			.25000-02	
3	0.1554	0.1977			.25000-02	
4	0.1581	0.1979			.25000-02	
5	0.1606	0.1981			.25000-02	
6	0.1000E-03	0.1981			.37600-01	.10000-03

ASPEN PLUS VER: DOS-386 REL: 8.4-1 INST: sjsu-utv 01/04/93 PAGE 39
D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
U-O-S BLOCK SECTION

BLOCK: 200DSTL MODEL: RADFRAC (CONTINUED)

			**** X-PROFILE ****
STAGE	C6H12	C7H8	
1	.13505	.86495	
2	.59669E-01	.94033	
3	.28994E-01	.97101	
4	.16785E-01	.98321	
5	.11755E-01	.98824	
6	.91635E-02	.99084	

			**** Y-PROFILE ****
STAGE	C6H12	C7H8	
1	.29980	.70020	
2	.12956	.87044	
3	.68199E-01	.93180	
4	.41811E-01	.95819	
5	.30482E-01	.96952	
6	.25245E-01	.97476	

			**** K-VALUES ****
STAGE	C6H12	C7H8	
1	2.2200	.80952	
2	2.5142	.90392	
3	2.6555	.95057	
4	2.7159	.97071	
5	2.7415	.97928	
6	2.7549	.98377	

BLOCK: 200SPLT MODEL: FSPLIT

INLET STREAM: 200PROD1
OUTLET STREAMS: 250FEED1 Z200TOPS
PROPERTY OPTION SET: SYSOP7 UNIFAC / REDLICH-KWONG

		*** MASS AND ENERGY BALANCE ***	
		IN	OUT
TOTAL BALANCE			RELATIVE DIFF.
MOLE(KMOL/HR)		0.500000E-01	0.500000E-01
MASS(KG/HR)		4.55317	4.55317
ENTHALPY(CAL/SEC)		9.34598	9.34598

*** INPUT DATA ***

MOLE-FLOW (KMOL/HR) STRM=250FEED1 FLOW= 0.0 KEY= 0

*** RESULTS ***

STREAM= 250FEED1 SPLIT= 0.0 KEY= 0
Z200TOPS 1.00000 0

0AFEED6 0AFEED5 0AFEED4 0AFEED3 0AFEED2

STREAM ID	0AFEED6	0AFEED5	0AFEED4	0AFEED3	0AFEED2
FROM :	----	----	----	----	----
TO :	OADSTL	OADSTL	OADSTL	OADSTL	OADSTL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	0.1163	1.5500-03	1.5500-03	1.5500-03	1.5500-03
C7H8	7.1288-02	9.5000-04	9.5000-04	9.5000-04	9.5000-04
TOTAL FLOW:					
KMOL/HR	0.1876	2.5000-03	2.5000-03	2.5000-03	2.5000-03
KG/HR	16.3576	0.2179	0.2179	0.2179	0.2179
L/MIN	0.3646	4.8594-03	4.8594-03	4.8594-03	4.8594-03
STATE VARIABLES:					
TEMP K	360.6406	360.6406	360.6406	360.6406	360.6406
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-1.9461+04	-1.9461+04	-1.9461+04	-1.9461+04	-1.9461+04
CAL/GM	-223.1918	-223.1918	-223.1918	-223.1918	-223.1918
CAL/SEC	-1014.1339	-13.5145	-13.5145	-13.5145	-13.5145
ENTROPY:					
CAL/MOL-K	-112.8901	-112.8901	-112.8901	-112.8901	-112.8901
CAL/GM-K	-1.2947	-1.2947	-1.2947	-1.2947	-1.2947
DENSITY:					
MOL/CC	8.5744-03	8.5744-03	8.5744-03	8.5744-03	8.5744-03
GM/CC	0.7476	0.7476	0.7476	0.7476	0.7476
AVG MW	87.1940	87.1940	87.1940	87.1940	87.1940

OAFEEED1 OAPROD1 OAPROD2 OAPROD3 OAPROD4

STREAM ID	OAFEEED1	OAPROD1	OAPROD2	OAPROD3	OAPROD4
FROM :	----	OADSTL	OADSTL	OADSTL	OADSTL
TO :	OADSTL	OBDSL	OBDSL	OBDSL	OBDSL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	MIXED	LIQUID
COMPONENTS: KMOL/HR					
C6H12	1.5500-03	1.9749-03	1.8288-03	1.7294-03	1.6598-03
C7H8	9.5000-04	5.2511-04	6.7115-04	7.7060-04	8.4017-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	2.5000-03	2.5000-03	2.5000-03
KG/HR	0.2179	0.2145	0.2157	0.2165	0.2171
L/MIN	4.8594-03	4.8585-03	4.8633-03	4.8613-03	4.8588-03
STATE VARIABLES:					
TEMP K	360.6406	357.3365	358.4048	359.1700	359.7256
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	4.1081-06	2.2581-06	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-1.9461+04	-2.6444+04	-2.4045+04	-2.2411+04	-2.1267+04
CAL/GM	-223.1918	-308.0743	-278.6122	-258.7255	-244.8936
CAL/SEC	-13.5145	-18.3642	-16.6981	-15.5633	-14.7690
ENTROPY:					
CAL/MOL-K	-112.8901	-124.6033	-120.5525	-117.8104	-115.8985
CAL/GM-K	-1.2947	-1.4516	-1.3968	-1.3600	-1.3345
DENSITY:					
MOL/CC	8.5744-03	8.5760-03	8.5676-03	8.5711-03	8.5754-03
GM/CC	0.7476	0.7361	0.7394	0.7424	0.7447
AVG MW	87.1940	85.8379	86.3040	86.6214	86.8434

OAPROD5 OAPROD6 OBPROD1 OBPROD2 OBPROD3

STREAM ID	OAPROD5	OAPROD6	OBPROD1	OBPROD2	OBPROD3
FROM :	OADSTL	OADSTL	OBDSL	OBDSL	OBDSL
TO :	OBDSL	OBDSL	OCDSL	OCDSL	OCDSL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	MIXED	MIXED
COMPONENTS: KMOL/HR					
C6H12	1.6069-03	0.1152	2.1597-03	2.0274-03	1.9053-03
C7H8	8.9309-04	7.2338-02	3.4027-04	4.7264-04	5.9467-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	0.1876	2.5000-03	2.5000-03	2.5000-03
KG/HR	0.2175	16.3659	0.2131	0.2141	0.2151
L/MIN	4.8591-03	0.3646	4.8591-03	4.8656-03	4.8704-03
STATE VARIABLES:					
TEMP K	360.1604	360.7606	356.0631	356.9660	357.8371
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	0.0	5.9388-06	1.0087-05
LFRAC	1.0000	1.0000	1.0000	0.9999	0.9999
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-2.0397+04	-1.9231+04	-2.9480+04	-2.7306+04	-2.5302+04
CAL/GM	-234.4177	-220.4387	-345.8193	-318.7371	-294.0025
CAL/SEC	-14.1647	-1002.1377	-20.4725	-18.9627	-17.5707
ENTROPY:					
CAL/MOL-K	-114.4477	-112.5076	-129.7829	-126.0669	-122.6699
CAL/GM-K	-1.3153	-1.2896	-1.5224	-1.4715	-1.4254
DENSITY:					
MOL/CC	8.5750-03	8.5742-03	8.5750-03	8.5635-03	8.5552-03
GM/CC	0.7461	0.7480	0.7310	0.7336	0.7362
AVG MW	87.0123	87.2386	85.2480	85.6704	86.0599

OBPROD4 OBPROD5 OBPROD6 OCPROD1 OCPROD2

STREAM ID	OBPROD4	OBPROD5	OBPROD6	OCPROD1	OCPROD2
FROM :	OBDSL	OBDSL	OBDSL	OCDSL	OCDSL
TO :	OCDSL	OCDSL	OCDSL	ODDSL	ODDSL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	MIXED
COMPONENTS: KMOL/HR					
C6H12	1.7949-03	1.6902-03	0.1144	2.2553-03	2.1491-03
C7H8	7.0509-04	8.0982-04	7.3116-02	2.4474-04	3.5093-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	0.1876	2.5000-03	2.5000-03
KG/HR	0.2160	0.2168	16.3721	0.2123	0.2132
L/MIN	4.8585-03	4.8587-03	0.3646	4.8595-03	4.8621-03
STATE VARIABLES:					
TEMP K	358.6622	359.4810	360.8501	355.4344	356.1339
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	0.0	0.0	2.6117-06
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-2.3488+04	-2.1766+04	-1.9060+04	-3.1050+04	-2.9305+04
CAL/GM	-271.8104	-250.9201	-218.4012	-365.5330	-343.6288
CAL/SEC	-16.3109	-15.1156	-993.2513	-21.5621	-20.3509
ENTROPY:					
CAL/MOL-K	-119.6155	-116.7320	-112.2245	-132.4917	-129.4823
CAL/GM-K	-1.3842	-1.3456	-1.2859	-1.5597	-1.5182
DENSITY:					
MOL/CC	8.5761-03	8.5756-03	8.5741-03	8.5743-03	8.5697-03
GM/CC	0.7410	0.7439	0.7482	0.7283	0.7308
AVG MW	86.4123	86.7466	87.2717	84.9431	85.2820

OCPROD3 OCPROD4 OCPROD5 OCPROD6 ODPROD1

STREAM ID	OCPROD3	OCPROD4	OCPROD5	OCPROD6	ODPROD1
FROM :	OCDSTL	OCDSTL	OCDSTL	OCDSTL	ODDSTL
TO :	ODDSTL	ODDSTL	ODDSTL	ODDSTL	ODDSTL
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	2.0328-03	1.9073-03	1.7676-03	0.1139	2.3096-03
C7H8	4.6722-04	5.9266-04	7.3244-04	7.3650-02	1.9038-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	2.5000-03	0.1876	2.5000-03
KG/HR	0.2141	0.2151	0.2162	16.3764	0.2119
L/MIN	4.8644-03	4.8677-03	4.8585-03	0.3646	4.8598-03
STATE VARIABLES:					
TEMP K	356.9283	357.8225	358.8725	360.9119	355.0846
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	4.9018-06	7.8586-06	0.0	0.0	0.0
LFRAC	1.0000	0.9999	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-2.7395+04	-2.5335+04	-2.3038+04	-1.8943+04	-3.1942+04
CAL/GM	-319.8392	-294.4076	-266.3391	-217.0016	-376.8148
CAL/SEC	-19.0244	-17.5936	-15.9987	-987.1431	-22.1822
ENTROPY:					
CAL/MOL-K	-126.2181	-122.7256	-118.8611	-112.0299	-134.0465
CAL/GM-K	-1.4736	-1.4261	-1.3741	-1.2833	-1.5813
DENSITY:					
MOL/CC	8.5656-03	8.5598-03	8.5760-03	8.5740-03	8.5737-03
GM/CC	0.7336	0.7366	0.7418	0.7484	0.7267
AVG MW	85.6531	86.0535	86.4996	87.2944	84.7696

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D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
STREAM SECTION

ODPROD2 ODPDOD3 ODPDOD4 ODPDOD5 ODPDOD6

STREAM ID	ODPROD2	ODPROD3	ODPROD4	ODPROD5	ODPROD6
FROM :	ODDSTL	ODDSTL	ODDSTL	ODDSTL	ODDSTL
TO :	OEDSTL	OEDSTL	OEDSTL	OEDSTL	OEDSTL
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	MIXED	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	2.2227-03	2.1166-03	1.9876-03	1.8269-03	0.1136
C7H8	2.7730-04	3.8338-04	5.1239-04	6.7315-04	7.4001-02
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	2.5000-03	2.5000-03	0.1876
KG/HR	0.2126	0.2134	0.2144	0.2157	16.3792
L/MIN	4.8611-03	4.8621-03	4.8642-03	4.8584-03	0.3646
STATE VARIABLES:					
TEMP K	355.6463	356.3525	357.2455	358.4198	360.9527
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	1.5299-06	2.7426-06	4.8002-06	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-3.0515+04	-2.8772+04	-2.6653+04	-2.4013+04	-1.8866+04
CAL/GM	-358.7970	-336.9690	-310.6552	-278.2125	-216.0818
CAL/SEC	-21.1907	-19.9807	-18.5093	-16.6754	-983.1271
ENTROPY:					
CAL/MOL-K	-131.5653	-128.5684	-124.9576	-120.4975	-111.9020
CAL/GM-K	-1.5469	-1.5057	-1.4564	-1.3960	-1.2816
DENSITY:					
MOL/CC	8.5714-03	8.5697-03	8.5660-03	8.5761-03	8.5740-03
GM/CC	0.7289	0.7317	0.7349	0.7402	0.7485
AVG MW	85.0470	85.3856	85.7973	86.3104	87.3094

OEPROD1 OEPROD2 OEPROD3 OEPROD4 OEPROD5

STREAM ID	OEPROD1	OEPROD2	OEPROD3	OEPROD4	OEPROD5
FROM :	OEDSTL	OEDSTL	OEDSTL	OEDSTL	OEDSTL
TO :	OFDSTL	OFDSTL	OFDSTL	OFDSTL	OFDSTL
SUBSTREAM: MIXED					
PHASE:	LIQUID	MIXED	MIXED	MIXED	MIXED
COMPONENTS: KMOL/HR					
C6H12	2.3421-03	2.2676-03	2.1699-03	2.0410-03	1.8681-03
C7H8	1.5793-04	2.3238-04	3.3012-04	4.5899-04	6.3192-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	2.5000-03	2.5000-03	2.5000-03
KG/HR	0.2116	0.2122	0.2130	0.2140	0.2154
L/MIN	4.8600-03	4.8609-03	4.8613-03	4.8626-03	4.8662-03
STATE VARIABLES:					
TEMP K	354.8783	355.3541	355.9950	356.8710	358.1112
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	1.1262-06	1.8513-06	3.3181-06	6.5689-06
LFRAC	1.0000	1.0000	1.0000	1.0000	0.9999
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-3.2476+04	-3.1253+04	-2.9647+04	-2.7530+04	-2.4690+04
CAL/GM	-383.5727	-368.0937	-347.9074	-321.5163	-286.4956
CAL/SEC	-22.5524	-21.7031	-20.5882	-19.1183	-17.1457
ENTROPY:					
CAL/MOL-K	-134.9807	-132.8442	-130.0696	-126.4483	-121.6376
CAL/GM-K	-1.5942	-1.5646	-1.5263	-1.4767	-1.4114
DENSITY:					
MOL/CC	8.5734-03	8.5718-03	8.5711-03	8.5689-03	8.5625-03
GM/CC	0.7258	0.7277	0.7303	0.7337	0.7379
AVG MW	84.6660	84.9036	85.2156	85.6269	86.1788

OEPROD6 OFPROD1 OFPROD2 OFPROD3 OFPROD4

STREAM ID	OEPROD6	OFPROD1	OFPROD2	OFPROD3	OFPROD4
FROM :	OEDSTL	OFDSTL	OFDSTL	OFDSTL	OFDSTL
TO :	OFDSTL	000DSTL	000DSTL	000DSTL	000DSTL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	MIXED	MIXED
COMPONENTS: KMOL/HR					
C6H12	0.1133	2.3619-03	2.2953-03	2.2033-03	2.0753-03
C7H8	7.4227-02	1.3811-04	2.0473-04	2.9671-04	4.2466-04
TOTAL FLOW:					
KMOL/HR	0.1876	2.5000-03	2.5000-03	2.5000-03	2.5000-03
KG/HR	16.3810	0.2115	0.2120	0.2127	0.2137
L/MIN	0.3646	4.8601-03	4.8608-03	4.8610-03	4.8618-03
STATE VARIABLES:					
TEMP K	360.9789	354.7532	355.1762	355.7738	356.6340
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	9.3601-07	1.4621-06	2.5719-06
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-1.8817+04	-3.2801+04	-3.1707+04	-3.0196+04	-2.8094+04
CAL/GM	-215.4923	-387.7088	-373.8315	-354.7899	-328.5211
CAL/SEC	-980.5526	-22.7786	-22.0185	-20.9693	-19.5099
ENTROPY:					
CAL/MOL-K	-111.8200	-135.5540	-133.6348	-131.0147	-127.4094
CAL/GM-K	-1.2805	-1.6022	-1.5756	-1.5393	-1.4898
DENSITY:					
MOL/CC	8.5739-03	8.5732-03	8.5719-03	8.5717-03	8.5702-03
GM/CC	0.7486	0.7253	0.7270	0.7295	0.7329
AVG MW	87.3190	84.6027	84.8154	85.1089	85.5173

OFPROD5 OFPROD6 000PROD1 000PROD2

STREAM ID	OFPROD5	OFPROD6	000PROD1	000PROD2	000PROD3
FROM :	OFDSTL	OFDSTL	000DSTL	000DSTL	000DSTL
TO :	000DSTL	000DSTL	050DSTL	050DSTL	050DSTL
SUBSTREAM: MIXED					
PHASE:	MIXED	LIQUID	LIQUID	MIXED	MIXED
COMPONENTS: KMOL/HR					
C6H12	1.8953-03	0.1132	2.3741-03	2.3124-03	2.2241-03
C7H8	6.0472-04	7.4369-02	1.2587-04	1.8762-04	2.7586-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	0.1876	2.5000-03	2.5000-03	2.5000-03
KG/HR	0.2152	16.3821	0.2114	0.2119	0.2126
L/MIN	4.8648-03	0.3646	4.8602-03	4.8608-03	4.8608-03
STATE VARIABLES:					
TEMP K	357.9106	360.9954	354.6764	355.0668	355.6369
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	5.3647-06	0.0	0.0	8.3088-07	1.2753-06
LFRAC	0.9999	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-2.5137+04	-1.8785+04	-3.3002+04	-3.1988+04	-3.0538+04
CAL/GM	-291.9763	-215.1197	-390.2654	-377.3888	-359.0948
CAL/SEC	-17.4561	-978.9250	-22.9182	-22.2137	-21.2071
ENTROPY:					
CAL/MOL-K	-122.3914	-111.7682	-135.9091	-134.1258	-131.6062
CAL/GM-K	-1.4216	-1.2799	-1.6071	-1.5824	-1.5475
DENSITY:					
MOL/CC	8.5650-03	8.5739-03	8.5731-03	8.5720-03	8.5719-03
GM/CC	0.7373	0.7487	0.7249	0.7265	0.7289
AVG MW	86.0920	87.3250	84.5637	84.7608	85.0424

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D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
STREAM SECTION

000PROD4 000PROD5 000PROD6 050PROD1

STREAM ID	000PROD4	000PROD5	000PROD6	050PROD1	050PROD2
FROM :	000DSTL	000DSTL	000DSTL	050DSTL	050DSTL
TO :	050DSTL	050DSTL	050DSTL	050SPLT	100DSTL
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	2.0970-03	1.9127-03	0.1131	4.8207-02	2.1785-03
C7H8	4.0296-04	5.8725-04	7.4458-02	4.2932-03	3.2151-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	0.1876	5.2500-02	2.5000-03
KG/HR	0.2136	0.2150	16.3829	4.4527	0.2129
L/MIN	4.8614-03	4.8640-03	0.3646	0.1020	4.8591-03
STATE VARIABLES:					
TEMP K	356.4855	357.7830	361.0058	355.1743	355.9377
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	2.1783-06	4.6759-06	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-2.8451+04	-2.5424+04	-1.8766+04	-3.1712+04	-2.9789+04
CAL/GM	-332.9594	-295.5002	-214.8858	-373.8927	-349.6795
CAL/SEC	-19.7574	-17.6553	-977.9036	-462.4596	-20.6864
ENTROPY:					
CAL/MOL-K	-128.0183	-122.8758	-111.7357	-133.6433	-130.3129
CAL/GM-K	-1.4982	-1.4281	-1.2794	-1.5757	-1.5297
DENSITY:					
MOL/CC	8.5709-03	8.5664-03	8.5739-03	8.5739-03	8.5749-03
GM/CC	0.7323	0.7370	0.7487	0.7271	0.7304
AVG MW	85.4480	86.0362	87.3288	84.8144	85.1881

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D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
STREAM SECTION

050PROD3 050PROD4 050PROD5 050PROD6

STREAM ID	050PROD3	050PROD4	050PROD5	050PROD6	100FEED1
FROM :	050DSTL	050DSTL	050DSTL	050DSTL	050SPLT
TO :	100DSTL	100DSTL	100DSTL	100DSTL	100DSTL
SUBSTREAM: MIXED					
PHASE:	MIXED	MIXED	MIXED	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	2.0272-03	1.8344-03	1.5983-03	6.8217-02	2.2956-03
C7H8	4.7281-04	6.6561-04	9.0173-04	6.9383-02	2.0444-04
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	2.5000-03	0.1376	2.5000-03
KG/HR	0.2141	0.2157	0.2176	12.1343	0.2120
L/MIN	4.8633-03	4.8618-03	4.8608-03	0.2676	4.8597-03
STATE VARIABLES:					
TEMP K	356.9672	358.3631	360.2324	363.5299	355.1743
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	3.9566-06	2.8101-06	1.3960-06	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-2.7303+04	-2.4136+04	-2.0255+04	-1.4344+04	-3.1712+04
CAL/GM	-318.7016	-279.7243	-232.7104	-162.6550	-373.8927
CAL/SEC	-18.9607	-16.7613	-14.0660	-548.2513	-22.0218
ENTROPY:					
CAL/MOL-K	-126.0620	-120.7056	-114.2110	-104.4341	-133.6433
CAL/GM-K	-1.4714	-1.3989	-1.3121	-1.1842	-1.5757
DENSITY:					
MOL/CC	8.5676-03	8.5703-03	8.5720-03	8.5683-03	8.5739-03
GM/CC	0.7339	0.7395	0.7461	0.7556	0.7271
AVG MW	85.6710	86.2863	87.0399	88.1853	84.8144

Z050TOPS 100PROD1 100PROD2 100PROD3

STREAM ID	Z050TOPS	100PROD1	100PROD2	100PROD3	100PROD4
FROM :	050SPLT	100DSTL	100DSTL	100DSTL	100DSTL
TO :	----	100SPLT	150DSTL	150DSTL	150DSTL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	MIXED	MIXED
COMPONENTS: KMOL/HR					
C6H12	4.5911-02	4.5124-02	1.9462-03	1.6926-03	1.3971-03
C7H8	4.0888-03	7.3764-03	5.5378-04	8.0739-04	1.1029-03
TOTAL FLOW:					
KMOL/HR	5.0000-02	5.2500-02	2.5000-03	2.5000-03	2.5000-03
KG/HR	4.2407	4.4773	0.2148	0.2168	0.2192
L/MIN	9.7194-02	0.1020	4.8696-03	4.8663-03	4.8640-03
STATE VARIABLES:					
TEMP K	355.1743	356.1362	357.5408	359.4616	362.0013
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	9.4119-06	6.3564-06	2.6910-06
LFRAC	1.0000	1.0000	0.9999	0.9999	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-3.1712+04	-2.9300+04	-2.5974+04	-2.1806+04	-1.6944+04
CAL/GM	-373.8927	-343.5611	-302.2664	-251.4025	-193.2490
CAL/SEC	-440.4378	-427.2908	-18.0372	-15.1433	-11.7669
ENTROPY:					
CAL/MOL-K	-133.6433	-129.4730	-123.8055	-116.7986	-108.7200
CAL/GM-K	-1.5757	-1.5181	-1.4407	-1.3465	-1.2399
DENSITY:					
MOL/CC	8.5739-03	8.5751-03	8.5565-03	8.5624-03	8.5664-03
GM/CC	0.7271	0.7313	0.7352	0.7426	0.7511
AVG MW	84.8144	85.2830	85.9294	86.7388	87.6818

100PROD5 100PROD6 150FEED1 Z100TOPS

STREAM ID	100PROD5	100PROD6	150FEED1	Z100TOPS	150PROD1
FROM :	100DSTL	100DSTL	100SPLT	100SPLT	150DSTL
TO :	150DSTL	150DSTL	150DSTL	----	150SPLT
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	1.0935-03	2.6898-02	2.1487-03	4.2975-02	2.9844-02
C7H8	1.4065-03	6.0702-02	3.5126-04	7.0251-03	2.2656-02
TOTAL FLOW:					
KMOL/HR	2.5000-03	8.7600-02	2.5000-03	5.0000-02	5.2500-02
KG/HR	0.2216	7.8569	0.2132	4.2641	4.5992
L/MIN	4.8656-03	0.1708	4.8590-03	9.7180-02	0.1020
STATE VARIABLES:					
TEMP K	365.0764	369.1159	356.1362	356.1362	361.7805
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	0.0	0.0	0.0
LFRAC	1.0000	1.0000	1.0000	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-1.1934+04	-6528.9023	-2.9300+04	-2.9300+04	-1.7340+04
CAL/GM	-134.6221	-72.7932	-343.5611	-343.5611	-197.9285
CAL/SEC	-8.2877	-158.8699	-20.3471	-406.9436	-252.8690
ENTROPY:					
CAL/MOL-K	-100.4834	-91.6885	-129.4730	-129.4730	-109.3733
CAL/GM-K	-1.1334	-1.0222	-1.5181	-1.5181	-1.2484
DENSITY:					
MOL/CC	8.5635-03	8.5465-03	8.5751-03	8.5751-03	8.5725-03
GM/CC	0.7591	0.7665	0.7313	0.7313	0.7510
AVG MW	88.6508	89.6910	85.2830	85.2830	87.6053

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D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
STREAM SECTION

150PROD2 150PROD3 150PROD4 150PROD5

STREAM ID	150PROD2	150PROD3	150PROD4	150PROD5	150PROD6
FROM :	150DSTL	150DSTL	150DSTL	150DSTL	150DSTL
TO :	200DSTL	200DSTL	200DSTL	200DSTL	200DSTL
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	MIXED	LIQUID	LIQUID
COMPONENTS: KMOL/HR					
C6H12	9.6003-04	6.0213-04	3.8459-04	2.7087-04	3.1146-03
C7H8	1.5400-03	1.8979-03	2.1154-03	2.2291-03	3.4485-02
TOTAL FLOW:					
KMOL/HR	2.5000-03	2.5000-03	2.5000-03	2.5000-03	3.7600-02
KG/HR	0.2226	0.2255	0.2272	0.2281	3.4396
L/MIN	4.8689-03	4.8826-03	4.9038-03	4.9039-03	7.3837-02
STATE VARIABLES:					
TEMP K	366.6233	371.5540	375.2776	377.5055	378.8538
PRES ATM	1.0000	1.0000	1.0000	1.0000	1.0000
VFRAC	0.0	0.0	6.7639-06	0.0	0.0
LFRAC	1.0000	1.0000	0.9999	1.0000	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-9724.1344	-3768.7208	-118.9475	1800.9406	2882.1717
CAL/GM	-109.1655	-41.7729	-1.3083	19.7306	31.5060
CAL/SEC	-6.7528	-2.6171	-8.2602-02	1.2506	30.1026
ENTROPY:					
CAL/MOL-K	-96.8758	-87.2364	-81.3987	-78.3585	-76.6597
CAL/GM-K	-1.0875	-0.9669	-0.8953	-0.8584	-0.8379
DENSITY:					
MOL/CC	8.5577-03	8.5337-03	8.4968-03	8.4966-03	8.4872-03
GM/CC	0.7622	0.7699	0.7724	0.7755	0.7764
AVG MW	89.0769	90.2192	90.9135	91.2764	91.4800

200FEED1 Z150TOPS 200PROD1 200PROD6

STREAM ID	200FEED1	Z150TOPS	200PROD1	200PROD6	250FEED1
FROM :	150SPLT	150SPLT	200DSTL	200DSTL	200SPLT
TO :	200DSTL	----	200SPLT	----	----
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	MIXED
COMPONENTS: KMOL/HR					
C6H12	1.4211-03	2.8423-02	6.7524-03	9.1635-07	0.0
C7H8	1.0789-03	2.1577-02	4.3248-02	9.9084-05	0.0
TOTAL FLOW:					
KMOL/HR	2.5000-03	5.0000-02	5.0000-02	1.0000-04	0.0
KG/HR	0.2190	4.3802	4.5531	9.2068-03	0.0
L/MIN	4.8605-03	9.7210-02	9.7975-02	1.9712-04	0.0
STATE VARIABLES:					
TEMP K	361.7805	361.7805	376.1717	383.2056	MISSING
PRES ATM	1.0000	1.0000	1.0000	1.0000	MISSING
VFRAC	0.0	0.0	0.0	0.0	MISSING
LFRAC	1.0000	1.0000	1.0000	1.0000	MISSING
SFRAC	0.0	0.0	0.0	0.0	MISSING
ENTHALPY:					
CAL/MOL	-1.7340+04	-1.7340+04	672.9107	6024.2710	MISSING
CAL/GM	-197.9285	-197.9285	7.3894	65.4329	MISSING
CAL/SEC	-12.0413	-240.8276	9.3459	0.1673	MISSING
ENTROPY:					
CAL/MOL-K	-109.3733	-109.3733	-80.1416	-71.8372	MISSING
CAL/GM-K	-1.2484	-1.2484	-0.8800	-0.7802	MISSING
DENSITY:					
MOL/CC	8.5725-03	8.5725-03	8.5055-03	8.4551-03	MISSING
GM/CC	0.7510	0.7510	0.7745	0.7784	MISSING
AVG MW	87.6053	87.6053	91.0634	92.0678	MISSING

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D&E 74, RR=3: 50KMOL/COL, HOLDUP, MEFF'CY=0.75
STREAM SECTION

Z200TOPS

STREAM ID Z200TOPS
FROM : 200SPLT
TO : ----

SUBSTREAM: MIXED

PHASE: LIQUID

COMPONENTS: KMOL/HR

C6H12 6.7524-03

C7H8 4.3248-02

TOTAL FLOW:

KMOL/HR 5.0000-02

KG/HR 4.5531

L/MIN 9.7975-02

STATE VARIABLES:

TEMP K 376.1717

PRES ATM 1.0000

VFRAC 0.0

LFRAC 1.0000

SFRAC 0.0

ENTHALPY:

CAL/MOL 672.9107

CAL/GM 7.3894

CAL/SEC 9.3459

ENTROPY:

CAL/MOL-K -80.1416

CAL/GM-K -0.8800

DENSITY:

MOL/CC 8.5055-03

GM/CC 0.7745

AVG MW 91.0634

APPENDIX B. COLLECTION of BATCH DISTILLATION SIMULATIONS

This appendix collects the data used to generate the plots in Chapters 3 and 4 and presents it in a standard format.

1. Published Simulations by Domenech & Enjalbert, Galindez & Fredenslund, Chiotti & Scenna for Domenech & Enjalbert's Case I: Reflux Ratio=3, Cyclohexane Feed Mol Fraction=0.62
2. Published Simulations by Domenech & Enjalbert [D9, D11], Galindez & Fredenslund [G2], Chiotti & Scenna [C1], Diwekar & Madhavan [D7] for Domenech & Enjalbert's [D9, D11] Case II: Reflux Ratio=4, Cyclohexane Feed Mol Fraction=0.55
3. Published Simulations by Domenech & Enjalbert, Galindez & Fredenslund, Chiotti & Scenna for Domenech & Enjalbert's Case III: Reflux Ratio=6, Cyclohexane Feed Mol Fraction=0.42
4. Published Simulations by Domenech & Enjalbert, Galindez & Fredenslund for Domenech & Enjalbert's Case IV: Reflux Ratio=5, Cyclohexane Feed Mol Fraction=0.30
5. Simulations using QSSCA, Plate-by-Plate Column Calculations and 2.5M/tray Holdup for Domenech & Enjalbert's Case I: Reflux Ratio=3, Cyclohexane Feed Mol Fraction=0.62
6. Simulations using QSSCA, Plate-by-Plate Column Calculations and 2.5M/tray Holdup for Domenech & Enjalbert's Case II: Reflux Ratio=4, Cyclohexane Feed Mol Fraction=0.55
7. Simulations using QSSCA, Plate-by-Plate Column Calculations and 2.5M/tray Holdup for Domenech & Enjalbert's Case III: Reflux Ratio=6, Cyclohexane Feed Mol Fraction=0.42
8. Simulations using QSSCA, Plate-by-Plate Column Calculations and 2.5M/tray Holdup for Domenech & Enjalbert's Case IV: Reflux Ratio=5, Cyclohexane Feed Mol Fraction=0.30

9. Simulations using QSSCA, Plate-by-Plate Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case I: Reflux Ratio=3, Cyclohexane Feed Mol Fraction=0.62
10. Simulations using QSSCA, Plate-by-Plate Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case II: Reflux Ratio=4, Cyclohexane Feed Mol Fraction=0.55
11. Simulations using QSSCA, Plate-by-Plate Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case III: Reflux Ratio=6, Cyclohexane Feed Mol Fraction=0.42
12. Simulations using QSSCA, Plate-by-Plate Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case IV: Reflux Ratio=5, Cyclohexane Feed Mol Fraction=0.30
13. Simulations using QSSCA, Short-cut Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case I: Reflux Ratio=3, Cyclohexane Feed Mol Fraction=0.62
14. Simulations using QSSCA, Short-cut Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case II: Reflux Ratio=4, Cyclohexane Feed Mol Fraction=0.55
15. Simulations using QSSCA, Short-cut Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case III: Reflux Ratio=6, Cyclohexane Feed Mol Fraction=0.42
16. Simulations using QSSCA, Short-cut Column Calculations and Neglecting Holdup for Domenech & Enjalbert's Case IV: Reflux Ratio=5, Cyclohexane Feed Mol Fraction=0.30

1. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case I: Reflux-Ratio=3, Feed $X_c=0.62$, Literature

2. Batch Distillation of Cyclohexane & Toluene

D&E (1974) Case II: Reflux-Ratio=4, Feed $X_c=0.55$, Literature

3. Batch Distillation of Cyclohexane & Toluene D&E (1974) Case III: Reflux-Ratio=6, Feed $X_c=0.42$, Literature

4. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case IV: Reflux-Ratio=5, Feed $X_c=0.30$, Literature

5. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case I: Reflux-Ratio=3, Feed $X_c=0.62$, Holdup=2.5M/tray

6. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case II: Reflux-Ratio=4, Feed $X_c=0.55$, Holdup=2.5M/tray

Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case III: Reflux-Ratio=6, Feed $X_c=0.42$, Holdup=2.5M/tray

8. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case IV: Reflux-Ratio=5, Feed $X_c=0.30$, Holdup=2.5M/tray

9. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case I: Reflux-Ratio=3, Feed $X_c=0.62$, Holdup=0.0M/tray

10. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case II: Reflux-Ratio=4, Feed $X_c=0.55$, Holdup=0.0M/tray

11. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case III: Reflux-Ratio=6, Feed $X_c=0.42$, Holdup=0.0M/tray

12. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case IV: Reflux-Ratio=5, Feed $X_c=0.30$, Holdup=0.0M/tray

13. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case I: Reflux-Ratio=3, Feed $X_c=0.62$, Edmister S'cut Calc'n

14. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case II: Reflux-Ratio=4, Feed $X_c=0.55$, Edmister S'cut Calc'n

15. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case III: Reflux-Ratio=6, Feed $X_c=0.42$, Edmister S'cut Calc'n

16. Batch Distillation of Cyclohexane & Toluene
D&E (1974) Case IV: Reflux-Ratio=5, Feed $X_c=0.30$, Edmister S'cut Calc'n

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