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Kerobo, Charles Omotayo

**FRACTIONATION OF MULTICOMPONENT MIXTURES BY STAGED
SEQUENCE CYCLIC PROCESS AND PARAMETRIC PUMPING**

New Jersey Institute of Technology

D.ENG.SC.

1982

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FRACTIONATION OF MULTICOMPONENT MIXTURES BY
STAGED SEQUENCE CYCLIC PROCESS AND
PARAMETRIC PUMPING —

by

Charles Omotayo Kerobo

Dissertation submitted to the Faculty of the Graduate School
of the New Jersey Institute of Technology in partial
fulfillment of the requirements for the degree of
Doctor of Engineering Science
1982

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 Mixtures by Staged Sequence Cyclic
 Process and Parametric Pumping

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"Research on Parametric Pumping," (with H.T. Chen, H.C. Hollein, and C.R. Huang), Chemical Engineering Education, Vol. 15, No. 4, Fall 1981.

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ABSTRACT

Title of Dissertation: Fractionation of Multicomponent Mix-
 tures by Staged Sequence Cyclic Pro-
 cess and Parametric Pumping

Charles Omotayo Kerobo, Doctor of Engineering Science, 1982

Dissertation directed by:

 Ching-Rong Huang
Professor and Assistant Chairman for Graduate Studies
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The continuous fractionation of multicomponent fluid mixtures has been experimentally and theoretically investigated by staged sequence cyclic process and parametric pumping operating in the direct thermal mode.

A multicolumn staged sequence cyclic process for the separation of solute mixtures was developed. The criteria necessary for the continuous fractionation of a system of n solutes with $n+1$ columns arranged in a series operated with $n+1$ cyclic variables is presented. The feasibility for practical application of this process was demonstrated by fractionating the model system, *o*-xylene-Anisole-*n*-heptane on silica gel. The separation was modeled by one column staged sequence experimental data and by the equations of continuity under nonequilibrium conditions with nonlinear equilibria of the individual solutes. Diverse operating variables necessary for maximum separation were optimized. The results showed that this process could be a viable alternative to parametric pumping, cycling zone adsorption, or simulated moving bed.

Two column parametric pumping arranged back-to-back with alternating top and bottom feed (to minimize reservoir mixing) was also used in the continuous fractionation of a model system consisting of toluene-acetophenone-n-heptane in silica gel. A simple method for predicting the purification of a given solute(s) was derived based on the method of characteristics, by assuming the existence of pseudo binary systems, each system consisting of one solute and the common solvent. Comparatively, two column parametric pumping provides better separation capability than a one column parapump.

PREFACE

A multicolumn staged sequence cyclic process for the continuous fractionation of solute mixtures has herein been introduced as a viable alternative to parametric pumping, cycling zone adsorption and simulated moving bed. A two column (back-to-back) parametric pumping process designed for the purification of solute mixtures, an extension of the state-of-the-art in separation processes, is also discussed. This advance will provide greater feasibility for practical application of these separation technologies.

DEDICATION

To the memory of Professor Hung-Tsung Chen, Educator, Advisor
and a true friend.

*If not for this or that
On such and such a day
Had varied by an hour or an inch
Or something neglected had been done
Or something done had been neglected*

Arthur Haley

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CHAPTER 1
INTRODUCTION & AN OVERVIEW OF CYCLIC
CHROMATOGRAPHIC SEPARATION PROCESSES

INTRODUCTION

Prior articles which describe the utility of single column or segmented column systems for cycling zone adsorption separation processes, as well as for comparable parametric pumping systems have herein been extended to multicolumn operations. This advance will provide greater feasibility for practical application of these separation technologies.

Direct thermal staged sequence cyclic separation processes and two column (effluent ends connected) back to back parametric pumping were investigated. The operating characteristics of two column and single column top feed (Chen, et al., 1972, 1973 and Stokes, 1976) parametric pumping processes were comparatively evaluated, and a limited comparison of parametric pumping versus staged sequence cyclic adsorption was made. The relative capabilities and performance characteristics of cycling zone and staged sequence cyclic process will be discussed.

Staged sequence adsorption and parametric pumping are cyclic separation processes characterized by unidirectional flow and flow reversal respectively, coupled to a change in a thermodynamic variable. The change in the intensive variable in a two phase system consisting of one mobile and one immobile phase (gas-solid, liquid-solid, or liquid-liquid) causes a separation

of the components to be achieved by alternately adsorbing and desorbing the solutes sequentially.

Various analytical solutions for the prediction of concentration histories are derived for chromatographic columns with step and pulse inputs based on linear or pseudo linear portions of non linear equilibria. These equations are useful for correlating system parameters that are necessary for design purposes. The theoretical prediction of the model with pulse inputs is applicable to the system in which the chromatographic column sequence consists of series of adsorption-desorption processes. The models of column operation range in complexity from that described by simplified equations of continuity to that describing a detailed and complex situation where in all the kinetic effects are taken into consideration. The derivations of these analytical solutions are covered in Chapter 3.

The analysis of direct thermal mode staged sequence adsorption and parametric pumping is based on equilibrium theory with linear and non linear equilibria as developed by Pigford (1969), as well as the more realistic non equilibrium theory with non linear equilibria of the favorable type. The equilibrium theory was generalized by Aris (1969) and applied to the analysis of continuous and semicontinuous single solute separation by Chen et al. (1972, 1973), and Gregory and Sweed (1970); and to multicomponent separation by Chen et al. (1974), Butts, Gupta, and Sweed (1972), and Foo, Bergsman and Wankat (1980). The nonequilibrium theory with non linear equilibria was first

applied to the analysis of parametric pumping by Wilhelm and his co-workers (1968).

The equilibrium theory assumes that the interface between the solid and the fluid phases are locally at equilibrium with a controlled linear distribution function having a temperature dependent equilibrium relationship. All diffusive and dispersive effects are assumed to be negligible. The equilibrium theory is most suitable for dilute solutions with linear equilibria, and is often extended to multicomponent systems by the principle of superimposition or by treating the multicomponent system as a series of pseudo-binary systems. The application of equilibrium theory to the staged sequence adsorption process and parametric pumping is covered in Chapters 4 and 5.

The non equilibrium approaches with linear and non linear equilibria constraints were simplified under the assumptions of constant fluid and solid properties, radial uniformity and negligible axial diffusion. In both cases, a linear interphase mass transfer rate was assumed. In the one case, the non-equilibrium with linear equilibria hypothetical treatment was solved by method of characteristics, while, in another case, the nonequilibrium with non linear equilibria was used to model the column by the STOP-GO algorithm (Sweed and Wilhelm, 1969) and is covered in Chapter 4.

AN OVERVIEW OF CYCLIC CHROMATOGRAPHIC SEPARATION PROCESSES

Cyclically operated gradient chromatographic processes are separation techniques characterized by unidirectional or alternating flow, coupled to a change in the thermodynamic variable. The change in the intensive variable induces separation of the components of a fluid mixture in a two-phase system consisting of one mobile and one immobile phase (gas-solid, liquid-solid or liquid-liquid). These cyclic processes include parametric pumping, pressure swing adsorption parametric pumping and cycling zone adsorption. In parametric pumping and pressure swing adsorption, the flow is alternating, while the flow in cycling zone adsorption is unidirectional. These new techniques in separation technology have received considerable attention in recent years.

Cyclic processes represent new developments in separation science because of both their novelty and their adaptability to techniques commonly used in the separation of fluid mixtures (i.e. adsorption, extraction, affinity chromatography and ion-exchange chromatography). The adaptation can be made, in principle, to any system where alteration of an applicable intensive variable such as temperature, pressure, pH, ionic strength or electric field results in a differential shift in the distribution of solutes between the mobile and immobile phases.

These new separation techniques have the following features:

- 1) batch chromatographic separations can be made semi-continuous or continuous; continuous operation minimizes processing time (thereby reducing degradation of sensitive substances like proteins) and maximizes production rate;
- 2) semi-continuous or continuous processes, when optimized, have high separation capabilities and the solutes can be concentrated within limits to desired levels by setting the relative volumes of the appropriate product streams;
- 3) no regeneration chemicals are needed to clean the adsorbents so chemical contamination of the product streams is eliminated.

The late Wilhelm and his co-workers (1966) invented the batch parapump and introduced a semi-continuous parapumping process. Since that time, a pre-existing industrial process known as "pressure swing adsorption" has been identified as operating on the parametric pumping principle. A similar process which utilizes cyclic variation of an intensive variable and unidirectional flow called "cycling zone adsorption" was developed by Pigford and his co-workers in 1969.

A brief mention will be made of separations resulting from cyclic changes in pressure and pH (with ionic strength or electric field). The brevity of the discussions that will be made on the aforementioned cyclic changes bears no reflection on the importance of these novel separation techniques, but is due

to their limited relevance to this study. However, thorough discussion will be offered on separations due to cyclic changes in temperature gradients.

PRESSURE SWING PARAMETRIC PUMPING

Pressure swing adsorption (or heatless adsorption as it is occasionally called) was invented by Skarstrom in 1959 who soon thereafter received the first U.S. patent on the process (in 1960). The experimental set-up consisted of a two column process which Skarstrom used alternating between adsorption at high pressure and desorption at low pressure employing an upward and downward flow of gas respectively. Shendalman and Mitchell (1972) presented the first detailed theoretical work on pressure swing adsorption using the model system CO₂-helium-silica gel. The configuration of their experimental set-up was similar to that of Skarstrom (1959). In their theoretical analysis, the equilibrium theory of Pigford (1969) was used, in which all of the dispersive forces were assumed negligible. Criteria necessary for good separation were developed, but their results did not agree both quantitatively and qualitatively. Mitchell and Shendalman (1973) presented a non-dispersive and non-equilibrium model in which equations were solved using finite difference technique by first reducing the equations from partial differential equations to ordinary differential equations by the method of characteristics.

Turnock and Kadlec (1971) studied the pressure swing adsorption processes for the separation of nitrogen and methane on

a molecular sieve. In the mathematical modeling of their system, instantaneous equilibrium, plug-flow, and ideal gas behavior were all assumed and the phase equilibria expression was assumed to obey the Freundlich isotherm. Their results agree both quantitatively and qualitatively with experimental determination. Kowler and Kadlec (1972) optimized the cycle time and found that in order to obtain the desired product composition and minimize the exhaust rate, an optimum cycle time of approximately three minutes was required. This work was also done using nitrogen and methane on a molecular sieve.

Jenczewski and Myers (1970) used an equilibrium model with favorable isotherm (Langmuir) to correlate experimental data from a closed thermal, pulse adsorber. At 15°C the active component is adsorbed, then the column temperature is increased to 70°C and the fluid is displaced by an amount equal to a fraction of the column void volume which was preselected before the start of the run. Three model systems were used--argon-propane, ethane-propane and propane-propylene--on activated carbon adsorbent. Measurable separation was not observed for the propane-propylene system. The separation observed for argon-propane and ethane-propane were quite poor. Radial temperature gradients of 1.0°C to 2.0°C were noticed even with the isothermal model of operation.

Lopez (1973) used an equilibrium plug-flow model for a batch isothermal system (propane-argon on activated carbon) using pressure swing adsorption. Effects of temperature, pressure and

concentration were investigated. A continuous pressure swing adsorption system was studied by Weingartner (1973) for the model system carbon dioxide-helium on silica gel. The experimental results were analyzed by means of an equilibrium theory, and the various operation parameters necessary for the complete removal of the solute (CO_2) were investigated.

Belsky (1977) extended the use of continuous pressure swing adsorption to the separation of a ternary mixture--propylene-carbon dioxide-helium on silica gel. Various performance characteristics were examined. Using the same model system, Rastogi (1977) experimentally and theoretically conducted a study based on a non-equilibrium theory and linear adsorption equilibria. A comparison was made for the binary and ternary gas mixtures, and the conditions necessary for the separation of multicomponent mixtures were established.

Chan et al. (1980) presented a theoretical analysis of pressure swing adsorption. The analysis was based on equilibrium theory for a two component system where the concentration of one component was assumed to be at trace level. The theory predicted that for a large separation factor, high recovery of pure product could be obtained and that increased pressure ratios should also increase the recovery. The converse was found true for small separation factors. The authors simplified the transport equations for the two components by assuming that the concentration of one of the components to maintain essential unity. By so doing, the two simultaneous equations were reduced

to one equation solvable by method of characteristics. Wong et al. (1980) studied the separation of hydrogen-tritium on vanadium hydride particles on a two column system. The mechanism of separation was evaluated theoretically and experimentally and they concluded that the separation was due to absorption isotope-effect which selectively occurred within the monohydride phase. Hill et al. (1982) conducted an experimental study with equipment similar to that of Wong et al. (1980), and modeled the separation by using equilibrium theory with minor modifications to include kinetic isotope effect, finite mass transfer and isotope exchange.

pH PARAMETRIC PUMPING (Fig. 1.1)

Parametric pumping processes, which are based on pH variation, are usually operated in the so-called recuperative mode, i.e. the intensive variable is set at a different level in the streams entering either end of the column. In this mode, the pH change moves across the bed as the entering streams penetrate the chromatographic column.

Sabadell and Sweed (1970) developed pH parametric pumping for the separation of aqueous solutions of K^+ and Na^+ on a cation exchange resin. The experimental apparatus was a one column arrangement with the top end open and the bottom end closed. Their results were rather encouraging since they were able to purify the material to 15 to 80% above the feed concentration. In 1975, Shaffer and Hamrin reported a pH parametric pumping process for trypsin removal from an enzyme mixture (chymo-

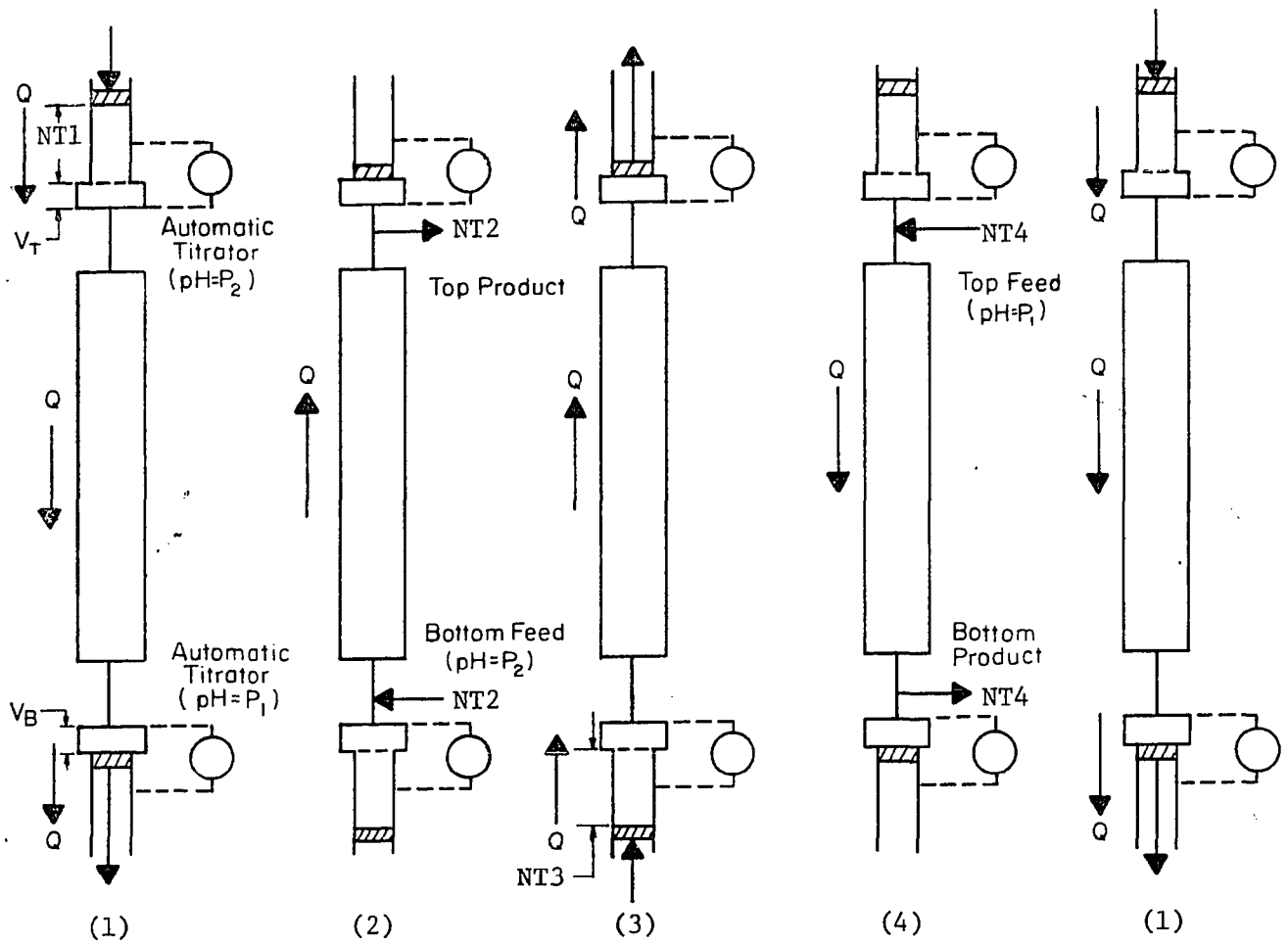


FIGURE 1.1 COLUMN DIAGRAM FOR CONTINUOUS pH PARAMETRIC PUMPING. (Kerobo, 1979)

trypsin plus trypsin) using a sepharose type ion exchanger. The separation was predicted by Pigford's (1969) equilibrium theory and the experimental results were much lower than the theoretical expectations. Since then, Chen and co-workers have researched protein separations via pH parametric pumping with emphasis on maximum separation and continuous operation.

Chen et al. (1976, 1977) have experimentally investigated a semi-continuous pH parametric pump using the model system of the two arbitrarily mixed proteins--human serum albumin and human hemoglobin in aqueous solution--on the sephadex cation exchanger. These two proteins have different isoelectric points and the processes developed for the model system may be applied to any mixture of proteins having different isoelectric points. Proteins which carry a net positive charge and will adsorb on a cation exchanger at pHs below their isoelectric points; proteins which carry a net negative charge adsorb at pHs above their isoelectric points. The semi-continuous pump, which had a center feed between an enriching column and a stripping column, was operated batchwise during upflow and continuously during downflow. Two pH levels were imposed periodically on the system. Various factors affecting the separation were examined, including pH levels and ionic strength of the protein solutions, reservoir displacement and product flow rates. Hemoglobin was stripped from the top stream and enriched in the bottom stream; the separation factor for hemoglobin reached a limit of six in the best run. The albumin concentration remains unchanged in

this process, but removal of hemoglobin from the top stream leaves the top product relatively richer (by weight fraction) in albumin.

Chen et al. (1979) used a continuous pH parametric pump to separate the model system hemoglobin-albumin on a CM sepharose cation exchanger. This pump configuration had protein feed solutions at low pH and at high pH (relative to the isoelectric point of hemoglobin) introduced respectively to the bottom and top of a chromatographic column. It was shown that increasing the volume of the top product to some optimum level relative to the volume of the bottom product gave the pump the capacity for large enrichment of hemoglobin in the bottom product stream. Note that this system should, in fact, be considered "semi-continuous," because each cycle contains two stages where the product is not withdrawn.

An equilibrium theory was used in a theoretical analysis of the batch single-column and multi-column pH parametric pump by Chen et al. (1980). Simple graphical procedures for predicting separation showed that a parametric pump consisting of a series of columns packed alternately with cation and anion exchangers is capable of yielding very high separation factors. Experimental results, based on a comparison of albumin enrichment in one column and two column systems packed with CM and DEAE sepharose, were shown to support the theory.

Chen et al. (1981) developed a mathematical model with finite mass transfer for the model system hemoglobin-albumin on

CM sepharose. This model agrees quite well with the experimental data. Various factors affecting the separation were examined, including the addition of recycle stages to the one column process.

Fractionation of multicomponent protein mixtures by multi-column pH parametric pumping was investigated theoretically and experimentally by Chen and co-workers (1980). The parametric pumping apparatus consisted of a series of chromatographic columns packed alternately with cation and anion exchangers. Separation of a mixture of n -proteins required a parametric pumping system consisting of n -columns and $n+2$ reservoirs. Various methods of operation of the parapump were discussed. Preliminary experimental data were shown in this paper for the two column batch separation of the model system hemoglobin-albumin on CM and DEAE sepharose, and these data were in qualitative agreement with the calculated results. Optimization of the batch two column system has been recently completed and separation factors as large as twenty five were obtained for the mixture (Chen et al., 1981).

OTHER RELATED VARIATIONS OF pH PARAMETRIC PUMPING

Chen, Ahmed and Rolian (1981) studied the purification of the enzyme (alkaline phosphatase) by parametric pumping with pH and ionic strength using a semi-continuous process. Alkaline phosphatase, extracted from the human placenta, contains some contaminating proteins which have isoelectric points approximately equal to that of the enzyme; hence, the additional

intensive variable (ionic strength). Comparison of enzyme purification by parametric pumping and cycling zone adsorption showed that the former process has a higher purification factor and a larger percentage enzyme activity recovered, while the latter process has a higher rate of production. Optimization indicated that a parametric pump operating with two proper combinations of the two intensive variables--pH and ionic strength--is superior to a parametric pumping system based on only pH or ionic strength.

Chen, Hollein and Ma (1981) have combined pH and electric field for splitting two proteins in a mixture from each other in a semi-continuous mode of operation with a single column set-up. The same model system was used as in previous protein separation studies, i.e. hemoglobin and albumin in aqueous solution on CM sepharose cation exchanger. The separation obtained in the single column, semi-continuous pH parametric pumping process is enhanced by inducing an electric field across the chromatographic column during certain stages of the process. Separation factors as high as 120 are reported for the mixture.

THERMAL PARAMETRIC PUMPING

The basic principles of parametric pumping were first described by Wilhelm et al. in 1966. In this pioneering work, a batch recuperative mode of operation was applied; the fluid was heated in a heat exchanger before flowing up through the bed and cooled before flowing down (see Figure 1.2a). Figure 1.2b illustrates the direct thermal mode batch parametric pumping

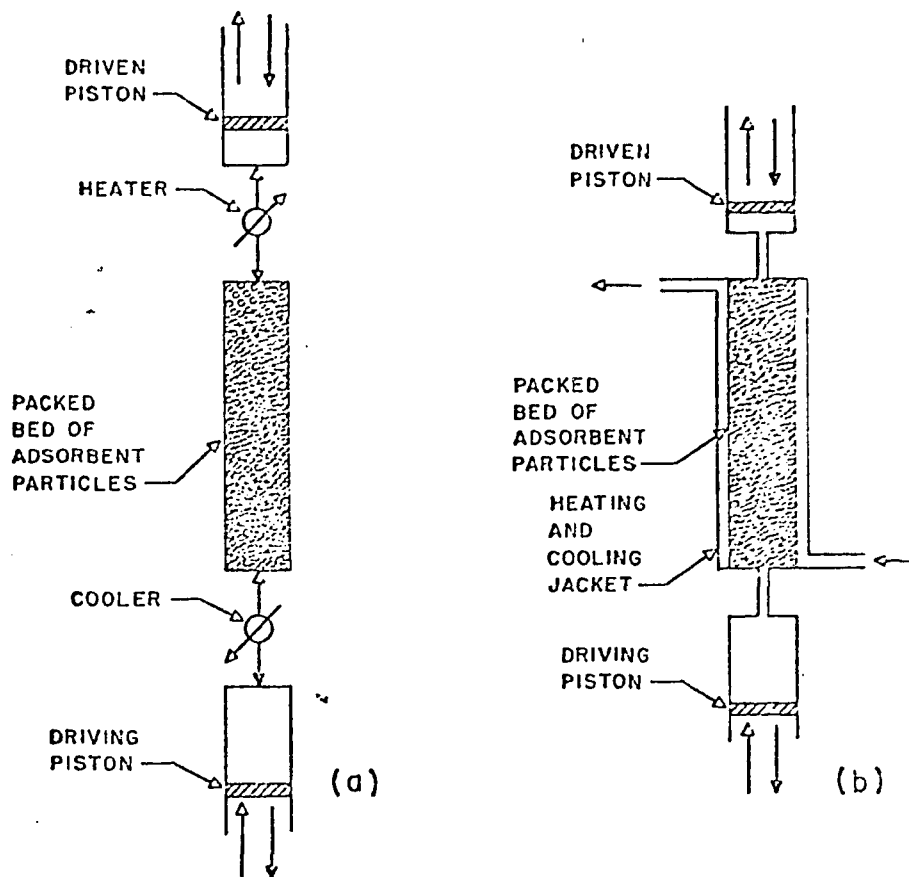


FIGURE 1.2 APPARATUS ARRANGEMENT FOR THERMAL PARAMETRIC PUMPING. (a) RECUPERATIVE MODE. (b) DIRECT MODE. (Wilhelm, 1966)

which calls for external application of heating and cooling sources during upward and downward flow of fluid through the column. The discussion of thermal parametric pumping will be started with the Direct Thermal Mode before going into the Recuperative Mode.

The Batch Direct Thermal Mode (Fig. 1.2b)

The direct thermal mode can further be subdivided into two categories, batch and open separations. The batch separations will first be presented in chronological order and followed then by the open separations. Briefly, a suitable experimental set up consists of a jacketed column packed with a suitable adsorbent. In the first half cycle, the column is heated and the fluid is flown from the bottom reservoir through the column to the top reservoir, and in the second half cycle, the column is cooled and the fluid is flown from the top reservoir through the column to the bottom reservoir. By successive synchronization of the flow directions with heating and cooling, the necessary separation is achieved. The principle behind the separation is that during the cold downflow, the adsorbent retains or retards the movement of the solutes, and releases them during the hot upflow, by so doing the solutes are concentrated at the top reservoir and depleted from the bottom reservoir.

The work of Wilhem and Sweed (1968) illustrates the batch direct thermal parametric pumping. The authors separated toluene from n-heptane on silica gel adsorbent employing two temperature cycling limits (hot and cold). The separation

factor (i.e. the ratio of the concentration in the top reservoir to the concentration in the bottom reservoir) was in the magnitude of $10^5:1$ after about 52 cycles. The theoretical method of analysis was complex and involves a good deal of computation. Sweed and Wilhelm (1969) presented a powerful method of computation algorithm for the solution of the transport equations resulting from the simulation of the batch pump. The equations are first simplified by reducing the partial differential equations to ordinary differential equations by method of characteristics, after which the ordinary differential equations are solved numerically by the STOP-GO method, suitable for handling of any rate equation. The method of characteristics eliminates all axial diffusion. The STOP-GO method was used to simulate the toluene-n-heptane data (Wilhelm and Sweed, 1968) and the comparisons were quite good.

Pigford, Baker and Blum (1969) developed the "equilibrium theory," based on the assumption of localized equilibrium between the solid and fluid phases. The material balance equations are greatly simplified since rate equations are not required. Linear equilibrium expression was assumed and all axial dispersive forces were neglected. The resulting equation after applying the assumptions is a hyperbolic equation solvable by method of characteristics. The validity of the equilibrium theory was tested by the authors by fitting the equilibrium parameter, b , with the data of Wilhelm et al. (1969), but no correlation was found, and, also, the concentrations are over

predicted. This lack of correlation, as one would expect, is a result of the oversimplification of the transport equations. In any case, this paper (Pigford et al. 1969) served as the limelight behind the reason for separation. The validity of the equilibrium theory caused considerable correspondence--amongst active and prominent investigators in this field--because of a difference of opinions. The equilibrium theory was generalized by Aris (1969). The prediction for low concentration was quite reasonable and the poor correlation for high concentration was attributed to mass transfer limitations.

To this reasoning, Rhee and Amundson (1979) pointed out that it was due to non-linear equilibria at high concentration rather than mass transfer resistances. Chen and Hill (1971) presented the separation characteristics of batch and open parametric pumping, the details of which will be discussed later. Sweed and Gregory (1971) modeled the separation of NaCl-H₂O-ion retardation resin. The dependence of mass transfer coefficients on temperature and velocity was determined from break through data. The data obtained from this work was used to simulate a continuous process. Butts, Gupta and Sweed (1972) used the equilibrium theory for the separation of multicomponent mixtures. The authors presented algebraic equations for the prediction of column and reservoir concentrations based on linear, non-competitive, non-dispersive and local equilibrium theory. The model considered asymmetric fluid displacements in both half cycles, thereby causing different solutes to penetrate dif-

ferent distances in the column. Butts et al. (1973) extended the analysis for multicomponent mixtures to the separation of a binary mixture of K^+ and H^+ on a Dowex 50x8 resin. K^+ ions were concentrated in the top reservoir and H^+ ions in the bottom reservoir. With slight modification in the operating conditions, a ternary mixture was separated. In this experiment, K^+ ion was concentrated in the top reservoir, H^+ in the bottom reservoir, and Na^+ in the middle of the column.

Gupta and Sweed (1973) used a mixing cell model to simulate the non-equilibrium effects in parametric pumping with linear isotherms. The effects of mass transfer resistances and axial diffusion were taken into consideration. This simulation is more realistic since equilibrium conditions are rarely attained in parametric pumping. The cell model was solved by either Laplace transform or matrix exponentiation. Grevillot and Tondeur (1976) studied equilibrium staged parametric pumps with non-linear isotherms. One single equilibration step and discrete transfer were regarded as one-half cycle. Suggestive analogies similar to that of total reflux distillation were given. Simple graphical McCabe-Thiele representation of the history of the concentration transients for the first few cycles was also presented. Single stage, two stage and nth stage parametric pumping were described. The number of stages is, in essence, equivalent to the number of cells. A one stage or cell means that the whole column, consisting of the adsorbent particle, is considered to be a single stage or cell. Grevillot and

Tondeur (1977) extended the single transfer step equilibrium graphical analysis (Grevillot and Tondeur, 1976) to multiple transfer equilibration steps per half-cycle. The reservoir concentrations were also embedded in the staging analysis. N equilibrium stage and n transfer steps per half cycle were also presented. The steady state graphical solution consists of a staircase for both linear and non-linear equilibria. Theoretically, increasing the number of transfer steps, n , even with a single stage, an infinite separation is possible, since the concentrations of the reservoirs are accounted for from cycle to cycle.

In a series of studies done by Rice and his co-workers (1973, 1973, 1974, 1975, 1975), qualitative treatment has been offered on batch parametric pumping. Their approach is a very important fundamental treatment that has been neglected since the inception of parametric pumping principles. Important dispersive forces that influence separation have been neglected for many years, all on the premise of simplifying the horror of mathematical equations resulting from modeling the internal and external solute movements in the column. Rice (1973) presented an analytical treatment for the prediction of the dispersive forces and steady state separation in parametric pumping. His derivation was based on "zero-flux condition," meaning that as the separation approaches a steady state value, the average solute flux approaches zero. The author also predicted that an optimum steady state separation occurs at a kinematic Peclet

number of about 3.0, and that larger separations could be obtained when the pump is operated at high frequency. Rice and Mackenzie (1973) presented experimental data for aqueous oxalic acid on activated carbon obtained from batch parametric pumping operated at high frequency. A reversed separation effect was observed. At high frequency of operation, thermal velocity is less than fluid velocity. Experimental studies on the temperature gradient showed that the variation of the axial temperature was in the neighborhood of 2°C. The author suggested inclusion of the radial diffusion terms in the original transport equations of Baker and Pigford (1971).

Rice and Foo (1974) studied the effects of thermal diffusion and frequencies of operation on batch parametric pumping operation. Rice and Mackenzie (1973) proved experimentally that axial temperature gradient was too small to be worthy of any attention in the modeling, but that radial thermal velocity is quite slow and could significantly affect the rate adsorption-desorption radially in the column. Rice (1974) studied the effects of all transport resistances on the optimum frequencies in parametric pumping. In commenting further on the temperature gradients in the column, the author assumed that small reservoir volumes are of sufficient physical grounds to neglect the axial temperature gradient, and that radial temperature gradients are primarily responsible for concentration dependence on radial position. Rice (1975) compared square velocity wave of Pigford (1969) to a sinusoidal velocity wave and concluded that para-

pumps operated with square velocity profiles produce larger separations than parapumps operated with purely sinusoidal velocity waves. For parapumps operated with equal displacements, but with square wave and sine wave velocity profiles, the author concluded that the enrichment of parapumps with sine wave velocity profile is slower.

The Continuous Direct Thermal Mode Parametric Pump (Fig. 1.3)

Application of the parametric pumping process to the separation of liquids in open systems has been studied extensively, both continuously and semicontinuously in the direct thermal mode. Sweed (1971) presented a considerable review of experimental work, while Horn and Lin (1969) were pioneers in presenting a theoretical calculation for such an open system. The experimental arrangement of Horn and Lin (1969) consisted of a two-column arrangement with a center feed, a center reservoir and reservoirs at both ends of the column where products were withdrawn. The mathematical description of the apparatus was rigorous. Firstly, a single solute system was used in which it was mathematically shown that the solute can be concentrated at one end of the reservoir (the "enrichment problem"). Secondly, the mathematical analysis of a two component "split problem" was also presented.

Gregory and Sweed (1970) introduced a continuous process analytically for an equilibrium parametric pump by method of characteristics. Separations resulting from symmetric and non-symmetric flow systems for various configurations are tabu-

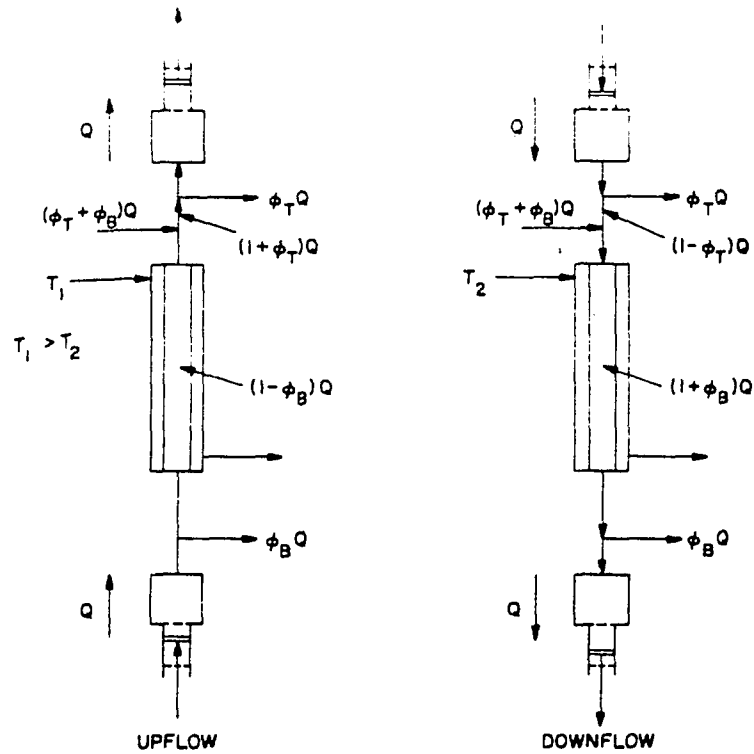


Fig. 1.3. Continuous Thermal Mode Parametric Pump with Top Feed (Chen and Hill, 1971)

lated. Sweed and Gregory (1971) simulated a continuous process with NaCl-H₂O-ion retardation resin system data obtained from a batch parametric pump. This paper was rather significant in that it illustrated that batch parametric pumping can be modeled accurately with a continuous process.

Chen and Hill (1971) introduced the first completely continuous parametric pumping process. Five different versions of the thermal parapump (two continuous, two semi-continuous, and the batch pump) were analyzed in terms of the equilibrium theory and the appropriate mass transport equations. The mathematical model indicates that, under certain operating conditions, the batch pump and pumps with feed at the enriched end have the capacity for complete removal of a solute from one product fraction and for arbitrarily large enrichment of that solute in the other fraction. Separation factors and enrichment are modest for pumps with feed at the depleted end. The concept of "penetration distance" was introduced in this paper as the distance a concentration front will move into the column during a half cycle. Experimental verification of these models for the system toluene-n-heptane on silica gel have been studied extensively by Chen and his co-workers (1972, 1973a, 1973b).

Chen et al. (1972) studied the continuous parapump operation experimentally with top feed. The system used for this continuous parapump was toluene-n-heptane on silica gel. A separation factor of over 600 was obtained for only 14 cycles in the region predicted by the equilibrium theory. In the initial work

done on the glucose-fructose-water system, fullers earth was used as the adsorbent (Chen, Jaferi and Stokes, 1972). The breakthrough data were fitted to a Langmuir isotherm and the separation predicted with equilibrium theory. A considerable attempt was made to design the experimental runs so that the equilibrium parameter, b , could be obtained. An extremely long cycle time was required for a typical run. Gregory and Sweed (1972) experimentally determined the behavior of a continuous parametric pumping system. Experimental batch data were used to simulate continuous process. Five versions of column arrangements were optimized. The equilibrium parameters and rates of mass transfer were experimentally determined and used in the solution of model equations by STOP-GO algorithm. Gupta and Sweed (1973) studied the effects of nonequilibrium in parametric pumping. The mixing cell model of a packed bed was used in the analysis of the nonequilibrium effects. The results obtained were more realistic when compared with the equilibrium theory. The authors presented a two column schematic for the separation of multicomponent mixtures by nonsymmetrical flow pattern in the columns.

A semicontinuous parametric pumping with top feed was experimentally studied by Chen, Reiss, Stokes and Hill (1973). Three possible regions of pump operations were presented. The concentration transient equations derived under equilibrium conditions were presented. It was postulated that an infinite steady state separation factor can be attained when the pump is

operated in Region 1 (separation factor equal the ratio of top product concentration to bottom product concentration). Chen and Manganaro (1974) derived mathematical expressions for determining optimal performance of equilibrium pumps. The studies were done with a model system $\text{NaNO}_3\text{-H}_2\text{O}$ via ion-retardation resin. Emphasis was placed on the operating conditions necessary for achieving high separation factors with maximum yield. Chen, Lin, Stokes and Fabisiak (1974) extended the continuous thermal parametric pumping to the separation of multicomponent mixtures. The model system used was toluene, aniline and n-heptane on silica gel. A simple method for predicting multicomponent separations was developed. This method invokes the assumption that a multicomponent mixture contains a series of pseudo-binary systems. Each binary system consists of one solute (toluene or aniline) plus the common inert solvent (n-heptane). Experimental data agreed reasonably well with the analytical predictions. The multicomponent system, glucose-fructose-water on a cation exchanger (Bio-Rad AG50W-X4, calcium form) was also studied (Chen and D'emidio, 1975). Agreement between experiment and theory was roughly equivalent to that obtained above.

In 1973, Sweed and Rigauudeau outlined the heat transfer problems that would be encountered in the scale up of thermal parametric pumping systems. The heating and cooling times are proportional to the diameter squared. The authors suggested packing numerous laboratory size tubes in a single shell for

scale up. A scale up of the continuous thermal parapumping system was done and the design equations were developed (Chen and Stokes, 1979). Proposals were outlined for the construction and operation of the parapump assembly; the auxiliary equipment and the instrumentation were also outlined. The commercial parapump assumes the configuration of multiple parallel tubes in a heat exchanger shell; this design facilitates direct thermal mode operation. The energy requirements were shown to be of the same order of magnitude as that for distillation.

Grevillot (1980) reported the analytical and theoretical equilibrium staged continuous parametric pumping process. This paper is an extension of two previous papers (1976, 1977) for the batch process. Operating conditions for a linear parapump are determined analytically and theoretically and generalized for non-linear isotherms. Analogies with distillation are made taking into account optimal feed stage location, minimum reflux and separation factor for given sets of conditions.

Rice and Foo (1981) carried out a direct-mode process for the continuous desalination of water using a dual-column system packed with bifunctional resin (Bio-Rad AG11A8). The derivations of the design equations for steady state continuous process were based on a nonequilibrium batch theory. The equation for the prediction of the steady state separation factor for continuous parapump as a function of the steady state separation factor for batch parapump and product rate seems to agree very well for the range of experiments undertaken.

Costa, Rodrigues, Grevillot and Tondeur (1982) have recently studied the purification of phenolic wastewater by a continuous direct mode parametric pumping using linear equilibrium theory. This work was done with a single column with top feed and packed with Duolite ES-681. The nonmixed dead volume model presented was tailored after the work of Chen and Hill (1971). The concentration transient equations developed to emphasize the influence of top and bottom dead volumes were also presented for batch, semicontinuous and continuous processes. Based on both of these experimental results and analytical results for the nonmixed reservoir, in order for the concentration transients to be improved, a minimum top dead volume should be maintained for a given bottom dead volume. Also, relative to the mixed case, a better separation could be obtained without top dead volume.

RECUPERATIVE THERMAL MODE PARAMETRIC PUMPING

In addition to the pH parametric pumping already discussed, the thermal recuperative mode was the first recuperative mode of parametric pumping initiated by Wilhelm and his co-workers (1966, 1968 and 1969). Despite the inherent energy recovery advantage of recuperative thermal mode over the direct thermal mode, much work has not been done in this area probably due to the difficulty of precise experimental work. The experimental results of Wilhelm and co-workers were rather discouraging. The separation factors that were obtained from their results ranged from an average value of 1.11 to a maximum value of 1.22.

However, Rolke and Wilhelm (1969) presented a very detailed mathematical modeling for the simulation of a continuous recuperative mode parametric pumping. Though the modeling was very attractive, the computational algorithm was too time consuming.

Sweed and Rigaudeau (1973) noticed that for there to be large separations, thermal waves must breakthrough the column for any given cycle. It was shown that earlier works on the recuperative mode were performed under the condition where thermal breakthrough did not occur. Simulated results where substantial separations could be obtained with proper selection of thermal penetration were also presented.

Wankat (1978) theoretically studied continuous thermal recuperative mode parametric pumping, and various conditions necessary to achieve complete and partial separation for a given solute from the bottom product were elaborated. When thermal wave velocity is greater than the concentration wave velocity, complete separation of solute from the bottom product is attained, and the separation for both direct and recuperative modes are the same. The energy requirements for a given separation are less for recuperative mode than direct mode, and could also be decreased for unmixed reservoirs. For pumps with partial separations, unmixed reservoirs could increase the separation.

A new concept recently presented by Tondeur, Jacob, Schweich and Wankat (1981) is the "Guillotine Effect." This effect, which is a result of thermal shock waves, would cause some solute

effluent concentrations to temporarily approach zero (very dilute). This phenomena could be noticed in any chromatographic adsorption-desorption process where pure cyclic thermodynamic waves can be obtained (i.e. temperature, pH and concentration). In fact, this phenomena is a result of adsorption of the solute due to a change in temperature from hot to cold. When the temperature is initially switched from hot to cold, the cold temperature front travels down the column; the solute concentration front trailing behind it is adsorbed, and, as the adsorbent capacity is approached, the solute concentration will rise and begin to approach the feed concentration.

CYCLING ZONE ADSORPTION

Cycling zone adsorption is a cyclic separation technique characterized by unidirectional flow through a series of columns called "zones." According to Pigford et al. (1969) who developed this process, the direct mode was called "standing wave," while the recuperative mode was called "travelling wave." In the direct mode, the columns are cooled or heated externally, and in the recuperative mode, the fluid entering the column is heated or cooled in a heat exchanger. The zones are arranged in a way such that the temperatures (or the applicable thermodynamic variables) are out of phase. The authors reported four experiments consisting of direct and recuperative mode of operation. Two of these experiments are single zone recuperative mode for the separation of methane from helium and acetic acid from water; while the other two experiments are a single zone direct mode for

the separation of acetic acid from water and double zone direct mode for acetic acid from water. The reported separation factors are high for the direct modes and even higher for the two zone. A detailed theoretical study was done by Baker and Pigford (1971), and theoretical explanation of the phenomena of separation of the cycling zone adsorption process presented. The authors showed that the equations applicable to the recuperative mode are equally applicable to the direct mode if the direct mode is considered to be a recuperative mode with infinite thermal wave velocity. The heat and mass balance equations were solved with the assumptions of local equilibrium theory (Pigford et al., 1969). The characteristic solution predicted that the cycling temperature on the column whether it was direct or recuperative, propagates through the column without changing shape or amplitude. The analytical solution for the linear isotherm predicts that infinite separation factors could be obtained as the number of zones approaches infinity, but similar conclusions cannot be reached for nonlinear isotherms due to shock and diffusive waves. The concentrations obtained for recuperative modes can be enhanced or amplified if the thermal wave velocity can be adjusted to be equal or lie between the concentration wave velocities of hot and cold temperatures. Experimental results of the adjustment of the thermal wave velocity was not reported.

Gupta and Sweed (1971) analyzed cycling zone adsorption process analytically. Model equations and graphical compu-

tational algorithms were presented based on equilibrium theory with linear equilibria. Their emphasis was on the proper selection of fluid displacement that would enable increased separation to be obtained. Ginde and Chu (1972) used a mixed bed of ion exchange resins in a single zone cycling adsorber to separate NaCl from water. This process was essentially a batch cycling zone with total recycle since products from the column were recycled until the desired separations were obtained. The parameters which affected separations were the amount of liquid in the system, the flow rate and the cycle time. In 1972, Rieke extensively studied the direct thermal mode of cycling zone adsorber for the model system toluene-n-heptane on silica gel. Experimental results showed that separation could be improved by switching temperature at an optimum frequency. Results for partial and no recycling were presented, and for the case with partial recycling, increased separation can be obtained, but longitudinal mixing limited the amount of separation.

Wankat (1973, 1974; see Fig. 1.4) extended the cycling zone adsorption process to liquid-liquid extraction. With a collection of test tubes, experiments were carried out for the separation of diethylamine-water-toluene, where toluene was used as the stationary phase. Direct and recuperative modes of operation were studied using the counter-current distribution system similar to that in Craig and Craig's "Technique of Organic Chemistry." Discrete transfer and equilibrium steps were applied to keep one liquid phase stationary. For the recuperative

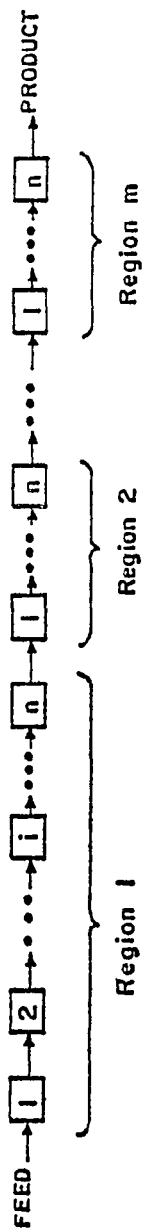


FIGURE 1.4 STAGED CYCLING ZONE EXTRACTION SYSTEM (Wankat, 1973)

mode, a dependency of separation on thermal wave velocity was observed. However, a qualitative agreement was obtained both theoretically and experimentally.

Meir and Lavie (1974) theoretically studied a continuous cyclic zone adsorption. In this recuperative mode process, a sinusoidal temperature input was assumed to be periodically imposed on the column. The mathematics of the problem was formulated under the assumption of local equilibrium. The analytical solution which was obtained via method of characteristics predicts the conditions under which separation could be obtained. Wankat (1975) showed that a recuperative mode cycling adsorption can be used to separate fluid mixtures into their individual components. The theoretical approach was based on local equilibrium and equilibrium staged theory. The temperature inputs consists of a series of temperature steps with one step for one component. Conditions necessary to effect separation were outlined. The equations presented were the same as those of Baker and Pigford (1971) and the conditions necessary for separation are based on the characteristic solution. The calculational scheme based on the equilibrium staged model is similar to the STOP-GO algorithm developed for parametric pumping (Sweed and Wilhelm, 1969).

Nelson, Silarski and Wankat (1978) developed a theoretical model for recuperative cycling zone adsorption processes. The equations were derived based on the equilibrium stage model and were solved numerically by the modified fourth order Runge-Kutta

method. The algorithm is a general scheme that is capable of handling different equilibrium isotherms and any thermodynamic intensive variable necessary for cyclic separations. The computer algorithm was used to simulate various experimental data and the results agree qualitatively. Foo, Bergsman and Wankat (1980) developed a segmented cycling zone adsorption system for the separation of multicomponent mixtures. This direct mode cycling zone system works on the principle that different solute concentration wave velocities have to be slower than or faster than given thermal wave velocities in order for the components to be separated. A single column consists of many zones and each zone consists of one or more sections. Based on the experimental results, the degree of separation depends on the total number of sections, the number of sections in a given temperature zone and the thermal switching rate.

CHAPTER 2
ADSORPTION MECHANISM IN PARAMETRIC PUMPING
AND CYCLIC ADSORPTION

The concept of adsorption chromatography is dated as far back as 1903 when it was first used for the separation of plant pigments. Since then, other analytical methods have been developed, and, as a result, the usage of adsorption chromatography has since been narrowed to the purification of fluid mixtures that are prohibitively expensive or impossible to separate by less conventional methods. This chapter will focus primarily on the adsorption of some organic compounds on some solid adsorbents.

The basic underlying principle of adsorption is interactions between the adsorbents (solid phase) and the adsorbates (solutes). These interactions can be purely physical, chemical or a combination of both. In physical adsorptions, layers of monomolecules are arranged on the adsorbent surface and are held there by weak van der Waals forces. Under appropriate operating conditions, the layers of monomolecules may concentrate at the interphase (interphase between the solid and fluid phases) due to these forces. The rate and degree of adsorption depends on the adsorbent type and the chemical properties of the adsorbates. On the other hand, chemisorption could involve reaction or chemical bonding between adsorbent and the adsorbate. The presence of the various forces in both the adsorbents and

adsorbates depends on their polarity (i.e. the positive and negative centers due to molecular arrangement or orientation).

Most adsorbents suitable for the separation of hydrocarbons may be polar (for adsorption chromatography) or non polar (for reverse phase partition chromatography). Silica gel, which was found most suitable for this study, is a polar adsorbent. The degree of adsorptive interactive forces will, in most part, increase with increased solute polarity. Solutes or solvents can be arranged in increasing order of dipole moment as follows:

Water > oxygenated organic compounds > hydrocarbons (2.1)

One can then conclude that the polarity of the solutes (solvents) increases with the number of assymmetrically placed functional groups, and decreases with increasing molecular weight for a given number of functional groups.

It is now evident that the adsorbent bed is the basis of chromatographic separation. So, to achieve separation, migration of substances through the bed has to be at different rates. The substances to be separated are passed through the adsorbent column and the adsorbent retarded or released based on the conditions of operation. The mobile phase serves as the avenue of transporting the solutes through the column. Therefore it will be very instructive to take a closer look at the stationary material and the way it selectively retards the solutes.

Figure 2.1 shows the chemical representation of the surface of silica gel. The basic germane characteristics of silica gel are the structure and chemical configuration of its surface.

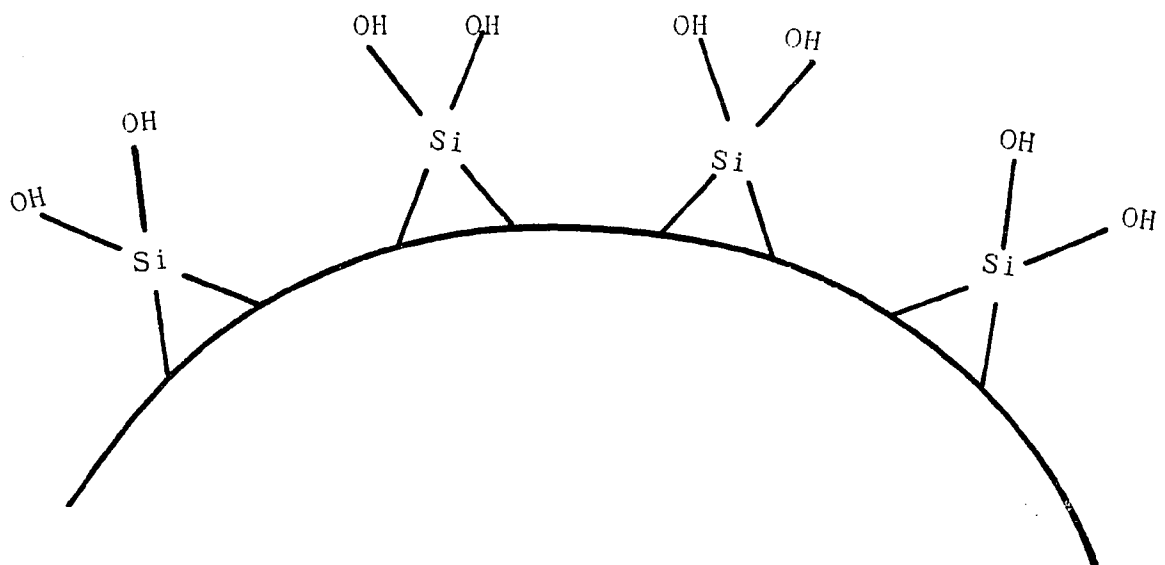


FIGURE 2.1 UNMODIFIED SILICA GEL

These surface characteristics can be exceedingly complex in nature. The surface layer can consist of hydrogen bonded water and silanol groups where one or two OH groups are attached to the same silicon atom. Silica gel can be chemically or thermally modified. If it is not chemically modified, there is a tendency towards irregularity in the number and spacing of the surface groups. The effect of these irregularities is a lack of reproducibility and separation characteristics. Silica gels that are not chemically modified have to be modified thermally (i.e. activation) so as to control the surface activity or strength. The number of OH groups accessible to the solutes determines the degree of bonding between the gel and the solutes. Silica gel can be partially or completely deactivated by the addition of water which covers the active sites by hydrogen binding. The importance of adsorbent selection to suit the material to be separated can not be overstressed. It is essential to have a thorough knowledge of the nature of the separation mechanism.

In adsorbents like silica gel, ion-dipole and dipole-dipole interactions may be responsible for the mechanism of adsorption. Induced dipole interactions (van der Waals forces) may also be present if materials to be separated are weakly polar. Amongst the various factors which may affect adsorption is the steric and spatial differences between solutes. This factor enables geometric and optical isomers to be separated by adsorption chromatography. The steric and spatial factors are also largely

responsible for the extent to which the solute is arranged on the surface of the adsorbents, and since some solutes are easily arranged relative to other solutes, the easily arranged solutes are adsorbed easily.

The usual configuration of a chromatographic process for the separation of liquid mixtures is a cylindrical column packed with pre-selected solid particles. In the convectional adsorption process, the fluid mixtures are introduced from the top of the column and the effluent collected in fractions and analyzed, or the compositions may be analyzed through an on-line system such as a gas chromatograph or UV spectrometer. As the fluid mixtures are steadily introduced, the solutes tend to be adsorbed by the solid, starting from the top of the column and gradually saturating the column as the process is continued. After saturation, the solutes are eluted by a single solvent, a combination of solvents or by applying an eluotropic series of solvents. The elution process depends on the solutes being separated. The packed column could be regenerated by heating, or, if the elution process consists of a rational series of solvents (Scott and Kucera, 1973), the packed column is automatically regenerated and ready for the next analysis. For processes that involve analytical separations, the fluid mixture is introduced in the form of a pulse followed by elution. The magnitude of the pulse input amongst many other factors depends on the purity desired.

EQUILIBRIUM CONSIDERATIONS

During the process of separation in a packed column, solute

bands migrate down the column at a velocity, $u_{i,con}$ (see Chapter 3). $u_{i,con}$, which is perhaps the major variable that ensures separability of different i solutes, is functionally dependent on the operating variables and equilibrium parameters.

$$u_{i,con} = f(\text{bulk velocity, solid phase concentration, thermodynamic variables, etc.}) \quad (2.2)$$

The equilibrium distribution between the solid and liquid phase can be expressed as

$$x_i = f(y, T) \quad (2.3)$$

Equation 2.3 means that the solid phase concentration, x , is functionally dependent on the liquid phase concentration, y , and the column temperature, T . The equilibrium distribution isotherms (Perry, 1973) are frequently characterized as "favorable" or "convex" (such as that shown in Figures 2.1 and 2.2) if, and only if

$$\frac{\partial^2 f}{\partial y^2} = \text{negative} \quad (2.4)$$

or "unfavorable" or "concave" if, and only if

$$\frac{\partial^2 f}{\partial y^2} = \text{positive} \quad (2.5)$$

and "linear" if, and only if

$$\frac{\partial^2 f}{\partial y^2} = \text{zero} \quad (2.6)$$

Favorable breakthrough curves such as that shown in Figures 2.1 and 2.2 can be calculated from unfavorable desorption data by the method of characteristics (Sherwood, Pigford and Wilke,

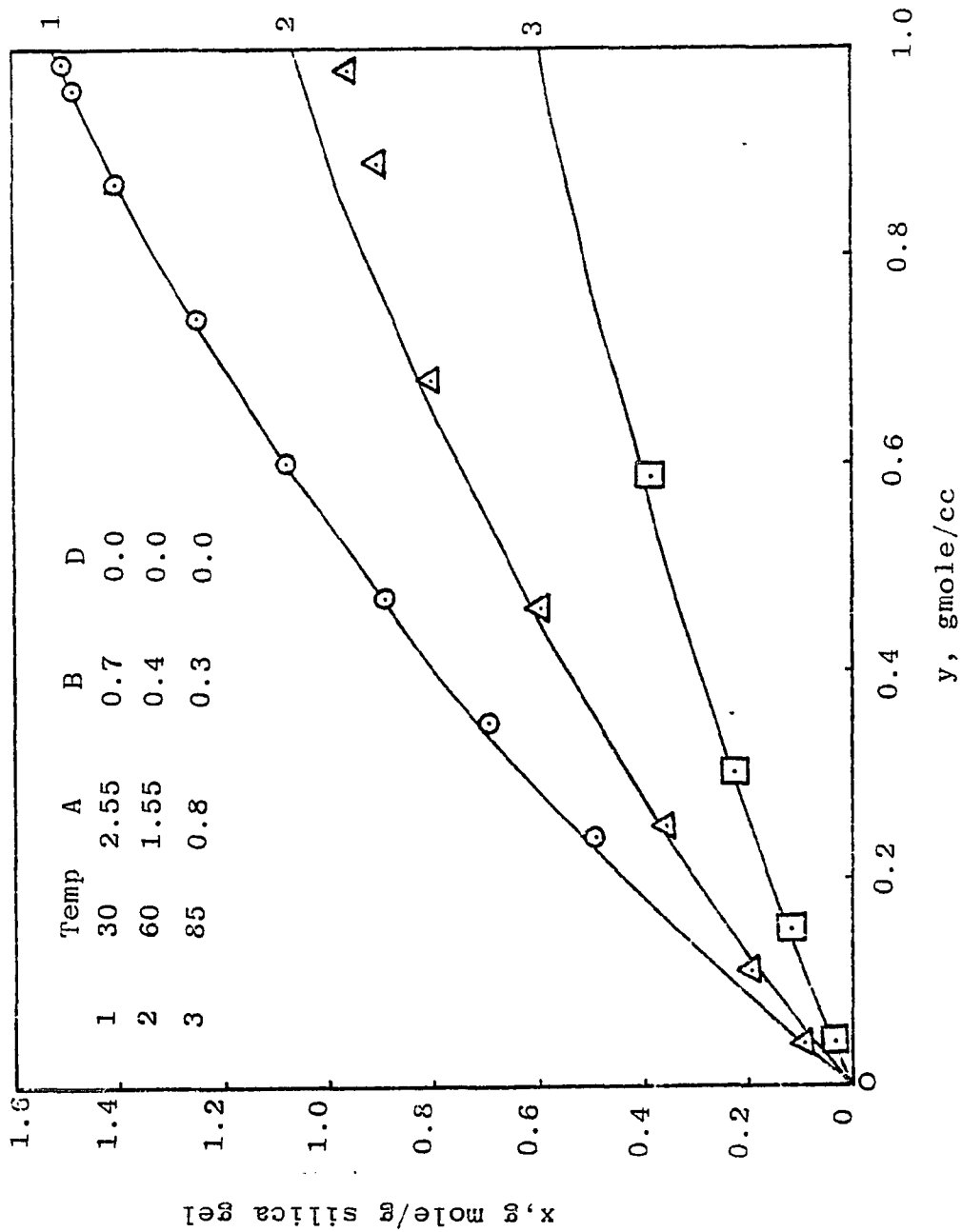


FIGURE 2.2 EQUILIBRIUM DISTRIBUTION ISOTHERM FOR O-XYLENE

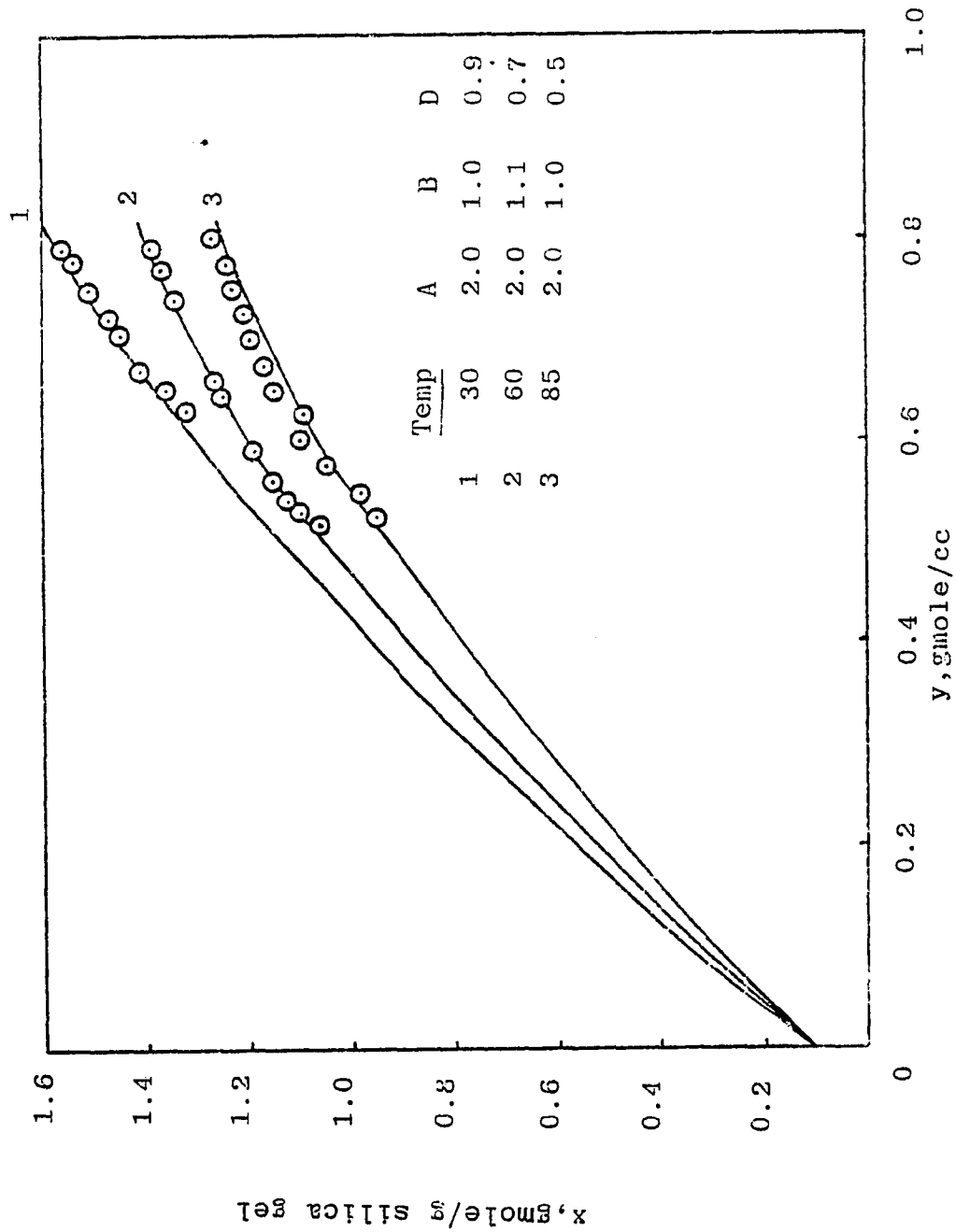


FIGURE 2.3 EQUILIBRIUM DISTRIBUTION ISOTHERM FOR ANISOLE

1975). Values of x , as a function of y , were estimated using desorption breakthrough data after the column was initially saturated by 1% v/v *o*-xylene and 1% v/v anisole in *n*-heptane. The column was eluted with pure *n*-heptane at a flow rate of 1 cc/min. This method of characteristics was derived for single solutes, but was extended to the analysis of two solutes by superposition of single solute results with the assumption that adsorption of each solute is independent of the presence of others. Equilibrium distribution isotherms for most solutes, especially hydrocarbons, exhibit convexity. There are few exceptions (Sherwood, Pigford and Wilke, 1975) to this observation in adsorption of electrolytic solutions in ion exchange resins. Contrary to most assumptions in the modeling of adsorptions in packed beds, linear equilibrium isotherms are not necessarily obtained at low (dilute) solute concentrations.

For qualitative and quantitative prediction of column behaviors, realistic expressions for the equilibrium distribution isotherm are imperative. This equilibrium distribution expression, which is the driving force, $F(x,y)$, that causes separation of solutes in a large number of packed columns, relates to the characteristic behavior of the solutes in both the liquid and solid phases. The most widely used of these adsorption equilibria expressions for single components are the famous Langmuir, Freundlich, Brunauer, Emmett, and Teller (BET) expressions, and for multicomponents the Langmuir expression. These are empirical correlations mostly derived for the adsorption of gas

mixtures (Sherwood, Pigford and Wilke, 1975) and have been successfully applied to the correlation of liquid mixtures.

The Langmuir expression (Eq. 2.7) was derived on the assumption of mono-layer and the fixed number of adsorption sites available for adsorption on the solid surface. Equation 2.7 is useful over a limited concentration range, and it also predicts linear equilibrium isotherms as the fluid phase concentration approaches zero.

$$x = \frac{QKy^*}{1 + Ky^*} \quad (2.7)$$

The Freundlich expression (Eq. 2.8) is the most widely used for the correlation of adsorption equilibria, but does not

$$x = ky^{1/n} \quad (2.8)$$

predict linear equilibrium isotherms as the concentration approaches zero. Other equilibrium isotherm expressions are extensions of the Langmuir isotherm developed for complex systems. For the systems used for this work, a modified Langmuir isotherm (first developed by Sweed, 1969) of the form

$$x = \frac{Ay^*}{1 + By^*} + Dy^* \quad (2.9)$$

was used. The constants A and B are temperature dependent constants to be determined empirically, while the constant D is dependent on the adsorbent type.

KINETIC CONSIDERATIONS

Although understanding of the kinetics of the movement of the solutes is a basic necessity for effective modeling of a packed bed, the transport mechanism of a given solute in a packed

bed could be very complex. A single or a combination of the following transport mechanisms contributes to the adsorption of the solute by the solid phase:

1. eddy diffusion;
2. mass transfer of the solute from the fluid phase to the interface;
3. mass transfer of the solute from the interface to the liquid phase;
4. mass transfer of the solute into the solid phase;
5. mass transfer of the solute on the adsorption sites of the solid phase; and
6. in some cases, chemical reaction of the solute with the adsorption sites.

During the process of adsorption, the above characteristic phenomena may be sequential as outlined and in the desorption process, the reverse order of the outlined sequence is true. For the formulation of simple models, most of the above mechanisms are neglected, especially the related mass-transfer resistances and longitudinal dispersion. And upon such simplifications, the concentration at the interphase is usually taken to be in equilibrium with the solid phase. The most frequently used models for the description of effluent curves from the packed bed are the equilibrium and finite mass transfer models.

In the equilibrium model, radial velocity, concentration, and temperature gradients are usually disregarded. In both isothermal and adiabatic operations, effect of temperature on

the physical parameters are usually neglected except in the equilibrium relationship. If mass transfer between the fluid and solid phases is assumed fast, simple adsorption equilibria may be adequate. The resulting transport equations, after applying the above assumptions, tend to overpredict the adsorption phenomena. However, it is advantageous in that the calculational algorithm involved is very simplistic in nature.

The finite mass transfer model tends to be more realistic in that solute mass transport across the interface is accounted for. For this model, the rate of mass transfer is due primarily to molecular diffusivity and convective forces. The rate of mass transport across the interface is usually expressed as

$$\frac{\partial x}{\partial t} = \lambda(y - y^*) \quad (2.10)$$

$$\lambda = \frac{ka}{1 - \epsilon} \quad (2.11)$$

$$k = [(1/K_f) + (1/K_s)]^{-1} \quad (2.12)$$

where

λ = overall mass transfer coefficient

k = overall mass transfer coefficient

K_f = fluid phase mass transfer coefficient

K_s = solid phase mass transfer coefficient

a = total interfacial area per unit volume of packed space

ϵ = column void volume fraction

For a slow rate of change of fluid and solid concentrations at the interface, the resistance to mass transfer is high and the contribution of solid phase mass transfer is negligible and $k = K_f$ (Eq. 2.12).

In equilibrium models with favorable distribution isotherms, the concentration wave front is concentration-dependent, and an influent of constant concentration causes a sharp concentration profile (Foo, Bergsman and Wankat, 1980; Helfferich and Klein, 1970)(i.e. discontinuous or shock front), and a step function is approached; whereas a diffuse wave is obtained for unfavorable distribution isotherms. For linear distribution isotherms the concentration wave front is concentration independent and influent of constant concentration displaces the wave front along the column with no change in shape.

The rate of advance of the solute concentration wave front can be expressed as (see Chapters 4 and 5)

$$u_{i,con} = \frac{v^e}{[\epsilon + (1 - \epsilon)f'(x_i, y_i)]} \quad (2.13)$$

and

$$f'(x_i, y_i) = \frac{\partial x_i}{\partial y_i}$$

where

v = the interstitial velocity of the solution; and

v^e = column superficial velocity.

For favorable distribution isotherms, $\partial x_i / \partial y_i$ decreases with y_i . This means that solute wave velocity is faster in the regions of high concentrations, and thereby overtakes a solute in a lower concentration region and a shock or sharp boundary results (Figure 2.4). Solutes with unfavorable distribution isotherm exhibit high velocities in the low concentration regions and diffuse waves result (Figure 2.4b), but the velocities of

solutes with linear isotherms are independent of concentration and thereby result in no change in solute wave fronts. The opposite phenomena takes place during a desorption process--solutes with favorable distribution isotherms exhibit diffuse waves, solutes with unfavorable distribution isotherms exhibit sharp or shock waves and those with linear distribution isotherms maintain constant shape concentration wave fronts.

From the ongoing analysis, it is evident that to design an efficient fixed bed or adsorption column, it is a matter of necessity to have a thorough understanding of adsorption mechanisms and the rate processes governing the system. Based on this understanding, the breakthrough curves (i.e. the effluent histories) can be logically analyzed. One shortcoming in the design of adsorption processes is that the rates and the mechanisms of the adsorption process are unique to the type of adsorption, the bulk fluid velocity, the concentration of the influent and the geometry of the adsorption column.

In the study of the dynamics of adsorption systems, the normal route generally taken is to predict the effluent history based on the influent history. Examples of influent histories commonly used are pulse and step inputs. Also, based on responses of the various inputs and the corresponding outputs, a suitable analysis and modeling of the system is done by formulating a mathematical representation to unify the relationships between the inputs and outputs. More often than not, the resulting equations may be so complex that in order for the

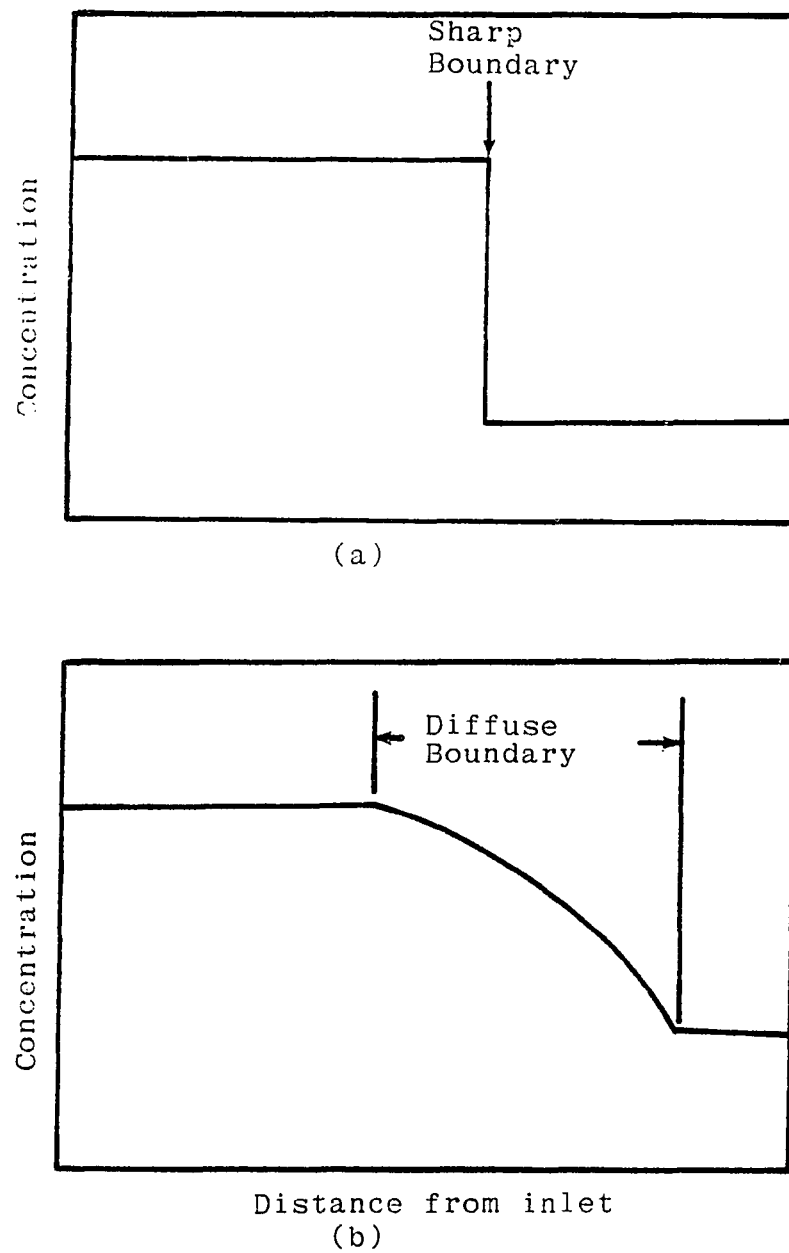


FIGURE 2.4 CONCENTRATION PROFILE WITH (a) SHARP BOUNDARY AND (b) DIFFUSE BOUNDARY

equations to be solvable, simplifying assumptions becomes a matter of course. Such studies where the solutes undergo adsorption and the effluents are continuously removed and analysis for concentration history have been elegantly described by Treybal ("Mass Transfer Operations") as "single transition systems." The single transition systems, as simple as it sounds, require a thorough knowledge for the interpretation and prediction of the effluent histories. Cyclic adsorption process and parametric pumping could be categorized as a "multiple transition system" since it involves an alternating series of adsorption and desorption. This means that a set of additional mathematical formulations is necessary for the prediction of the desorption process. The adsorption and desorption steps in cyclic adsorption and parametric pumping involves a change in the intensive variable such as temperature, pressure, pH, ionic strength, electric field or magnetic field. The alteration of the intensive variable results in a differential shift in the distribution of solutes between the mobile and immobile phases. By taking into account the effects of the various or appropriate intensive variable, the mathematical modeling is further complicated.

CHAPTER 3

THE MATHEMATICS OF ADSORPTION IN A PACKED BED

THE COMPLETE MODEL OF A PACKED BED

The packed bed under consideration is assumed to have a cross sectional area of S square units. It is also assumed that it is packed with fine particles such that the void volume is filled with solvent or solution. At time zero, a solution of known concentration is pumped into the column at room temperature and the column itself is operated isothermally at known temperature T . It is assumed that the process of adsorption of all solutes is non-competitive. It is desired to determine the fluid phase concentration at any time and at any position in the bed.

Then making a detailed material balance on an elemental length of bed ΔZ (Figure 3.1), the following result was obtained:

Fluid Phase

$$\begin{aligned} \epsilon S \Delta z \frac{\partial y}{\partial t} &= v S y|_{z=z} - v S y|_{z=z+\Delta z} \\ &- \frac{S \Delta z (1 - \epsilon)}{4/3 \pi r_o^3} \cdot 4 \pi r_o^2 K_f (y - y_{int}) \\ &- \epsilon S E_D \frac{\partial y}{\partial z} \Big|_{z=z} + \epsilon S E_D \frac{\partial y}{\partial z} \Big|_{z=z+\Delta z} \end{aligned} \quad (3.1)$$

dividing Eq. 3.1 by $\Delta z \epsilon S$, as Δz approaches 0, we get

$$\frac{\partial y}{\partial t} = - \frac{v}{\epsilon} \frac{\partial y}{\partial z} - \frac{1 - \epsilon}{\epsilon} \frac{3}{r_o} K_f (y - y_{int}) + E_D \frac{\partial^2 y}{\partial z^2} \quad (3.2)$$

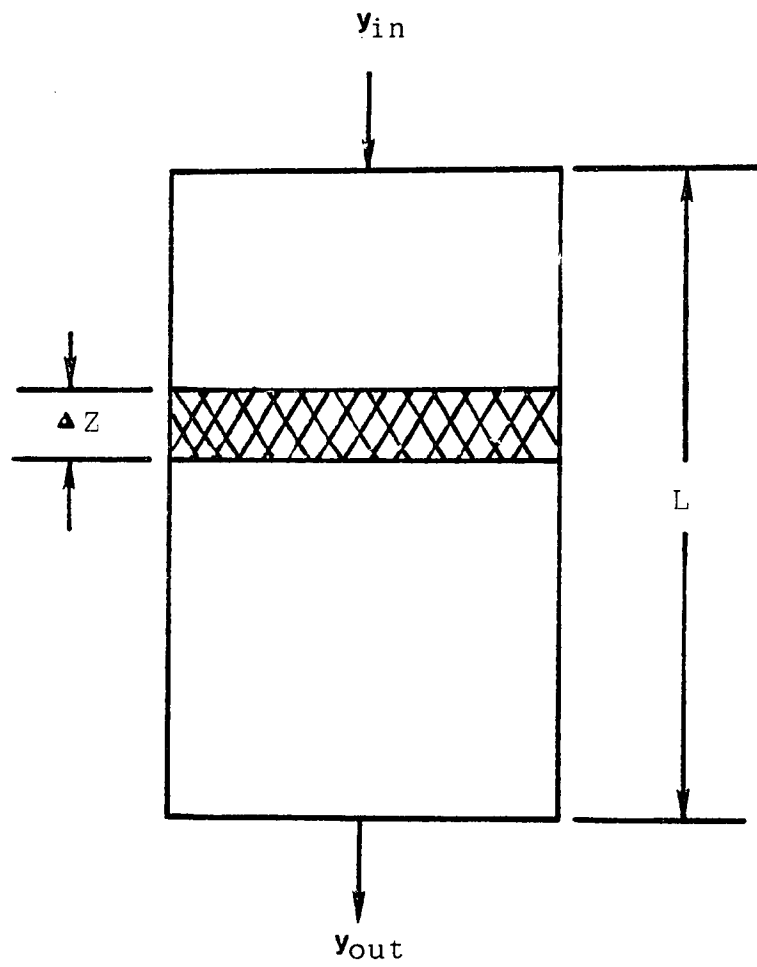


FIGURE 3.1 FIXED BED PACKED WITH ADSORBENT PARTICLES

Solid Phase

$$4\pi r^2 \cdot N_{Ar}|_r - 4\pi r^2 N_{Ar}|_{r+\Delta r} = 4\pi r^2 \cdot \Delta r \cdot \frac{\partial x}{\partial t} \quad (3.3)$$

dividing Eq. 3.3 by $4\pi\Delta r$, as Δr approaches 0, we get

$$-\frac{\partial (r^2 N_{Ar})}{\partial r} = r^2 \frac{\partial x}{\partial t} \quad (3.4)$$

Since $N_{Ar} = -D_S \frac{\partial x}{\partial r}$, Eq. 3.4 becomes

$$D_S \left(r^2 \frac{\partial^2 x}{\partial r^2} + 2r \frac{\partial x}{\partial r} \right) = r^2 \frac{\partial x}{\partial t} \quad (3.5)$$

For spherical particles, the particle shape factor $\alpha_f=2$. Therefore upon rearrangement of Eq. 3.5, we get

$$D_S \left(\frac{\partial^2 x}{\partial r^2} + \frac{\alpha_f}{r} \frac{\partial x}{\partial r} \right) = \frac{\partial x}{\partial t} \quad (3.6)$$

To understand the mechanism of adsorption, some assumptions are necessary. The relationship between the fluid phase, y , and the solid phase, x will be assumed to be linear. The constraint that goes with this assumption requires that we stay within the dilute concentration region. If we invoke the local equilibrium theory of Pigford et al. (1969), we have in the region of small $x(r=r_0)$

$$y_{int}(z, t) = Kx(r = r_0, z, t) \quad (3.7)$$

Equation 3.7 implies that equilibrium is established at every time and space in the bed. K is a function of the intensive variable (e.g. temperature, pressure, pH, etc.) and all the flow characteristics of the bed. The initial conditions of the bed are:

$$y(z, t = 0) = y_0 = \text{constant}, 0 \leq z \leq L \quad (3.8)$$

which also means that $y_{\text{int}}(z, t = 0) = y_0$

$$x(r, z, t = 0) = x_0 = \text{constant}, 0 \leq z \leq L, 0 \leq r \leq r_0 \quad (3.9)$$

The boundary conditions necessary for a complete solution are

$$\frac{v}{\epsilon} y(z = 0, t) - E_D \left. \frac{\partial y(t)}{\partial z} \right|_{z=0} = \frac{v}{\epsilon} y_{\text{in}} \quad (3.10)$$

$$\left. \frac{\partial y}{\partial z} \right|_{z=L} = 0 \text{ for small } t, y = y_0 \quad (3.11)$$

$$y(z = L, t) = y_{\text{in}} \text{ for large } t, y = y_{\text{in}} \quad (3.12)$$

$$\left. \frac{\partial y}{\partial z} \right|_{z=L} = \text{finite for intermediate } t \text{ or } \left. \frac{\partial^2 y}{\partial x^2} \right|_{z=L} = 0 \quad (3.13)$$

Equations 3.11 through 3.13 can be combined to give

$$\left. \frac{\partial^2 y}{\partial z^2} \right|_{z=L} = 0 \quad (3.14)$$

$$\left. \frac{\partial x}{\partial r} \right|_{r=0} = 0 ; 0 \leq z \leq L, t \geq 0 \quad (3.15)$$

$$D_S \left. \frac{\partial x}{\partial r} \right|_{r=r_0} = K_f [y(z, t) - y_{\text{int}}(r_0, z, t)] \\ 0 \leq z \leq L, t \geq 0 \quad (3.16)$$

$y_{\text{int}}(r_0, z, t) = f[x(r_0, z, t)]$ as shown by Eq. 3.7

$$y(z, t \rightarrow \infty) = y_{\text{in}} \quad (3.17)$$

$$x(r_0, z, t \rightarrow \infty) = x_{\text{eq}} = \frac{y_{\text{int}}}{K} = \frac{y_{\text{in}}}{K} \quad (3.18)$$

Equations 3.2 and 3.6 become

$$\frac{\partial Y}{\partial t} + \frac{(1 - \epsilon)}{\epsilon} \cdot \frac{3}{r_0} \cdot K_f(Y - Y_{int}) = E_D \frac{\partial^2 Y}{\partial z^2} - \frac{v}{\epsilon} \frac{\partial Y}{\partial z} \quad (3.19)$$

and

$$\frac{\partial X}{\partial t} = D_S \left(\frac{\partial^2 X}{\partial r^2} + \frac{2}{r} \frac{\partial X}{\partial r} \right) \quad (3.20)$$

where

$$Y = -(y - y_0), \quad Y_{int} = -(y_{int} - y_0)$$

and

$$X = -(x - x_0)$$

Note that as y increases with respect to t , and decreases with respect to z ; Y decreases with respect to time t , and increases with respect to z . So also x increases with respect to r and t ; and X decreases with respect to r and t .

Laplace transform Eq. 3.20, with Eq. 3.9 to get

$$S\bar{X} = D_S \left(\frac{d^2 \bar{X}}{dr^2} + \frac{2}{r} \frac{d\bar{X}}{dr} \right) \quad (3.21)$$

or

$$r^2 \frac{d^2 \bar{X}}{dr^2} + 2r \frac{d\bar{X}}{dr} - \frac{S}{D_S} r^2 \bar{X} = 0 \quad (3.22)$$

Equation 3.22 is a Bessel equation. The generalized Bessel's equation is of the form

$$x^2 \frac{d^2 y}{dx^2} + x(a + 2bx^r) \frac{dy}{dx} + [c + dx^{2N} - b(1 - a - r)x^r + b^2 x^{2r}] y = 0 \quad (3.23)$$

The general solution to Eq. 3.23 is

$$y = x^{\frac{1-a}{2}} \cdot e^{-\frac{bx^r}{r}} \left[c_1 Z_p \left(\frac{\sqrt{|d|}}{N} x^N \right) + c_2 Z_{-p} \left(\frac{\sqrt{|d|}}{N} x^N \right) \right] \quad (3.24)$$

where

$$p = \frac{1}{N} \sqrt{\left(\frac{1-a}{2}\right)^2 - c}$$

For the problem at hand, $a = 2$, $b = 0$, $d = -\frac{N}{DS}$, and $N = 1$

$$p = \frac{1}{1} \sqrt{\left(\frac{1-2}{2}\right)^2} = \frac{1}{2}$$

Therefore,

$$\bar{X} = r^{-\frac{1}{2}} \left[c_1 I_{\frac{1}{2}}\left(\sqrt{\frac{S}{DS}} r\right) + c_2 I_{-\frac{1}{2}}\left(\sqrt{\frac{S}{DS}} r\right) \right] \quad (3.25)$$

From Eq. 3.15

$$x(r = 0, z, t) = \text{finite, at } r = 0 \quad (3.26)$$

The Laplace transform of Eq. 3.26 is

$$\bar{X} = \text{finite at } r = 0 \quad (3.27)$$

Application of Eq. 3.27 to Eq. 3.25, gives

$$C_2 = 0$$

and

$$\bar{X} = C_1 r^{-1/2} I_{1/2}\left(\sqrt{\frac{S}{DS}} r\right) \quad (3.28)$$

because

$$I_{1/2}\left(\sqrt{\frac{S}{DS}} r\right) \cong \frac{\left(\frac{S}{DS}\right)^{1/4}}{2^{1/2} \cdot (1/2)!} r^{1/2} \text{ for small } r$$

and

$$I_{-1/2}\left(\sqrt{\frac{S}{DS}} r\right) \cong \frac{2^{1/2}}{(-1/2)!} \left(\frac{S}{DS}\right)^{-1/4} \cdot r^{-1/4} \text{ for small } r$$

one should also note that

$$c_1 = f(z) \text{ since } x = f(r, t)$$

so

$$X = f(r, t) \quad \text{and} \quad \bar{X} = f(r, S)$$

Take the derivative of Eq. 3.28

$$\frac{\partial \bar{X}}{\partial r} = C_1 \sqrt{\frac{S}{D_S}} \cdot r^{-1/2} \cdot I_{3/2}\left(\sqrt{\frac{S}{D_S}} r\right)$$

since

$$\frac{d}{dx} [x^{-P} I_P(\alpha x)] = \alpha x^{-P} I_{P+1}(\alpha x)$$

Therefore

$$\left. \frac{\partial \bar{X}}{\partial r} \right|_{r=r_0} = C_1 \sqrt{\frac{S}{D_S}} r_0^{-1/2} \cdot I_{3/2}\left(\sqrt{\frac{S}{D_S}} r_0\right) \quad (3.29)$$

Take Laplace transform of Eq. 3.19 with the initial condition of Eq. 3.8 to get

$$S\bar{Y} + \frac{(1 - \epsilon)}{\epsilon} \cdot \frac{\alpha_f + 1}{r_0} K_f(\bar{Y} - \bar{Y}_{int}) = E_D \frac{d^2 \bar{Y}}{dz^2} - \frac{v}{\epsilon} \frac{d\bar{Y}}{dz} \quad (3.30)$$

Take Laplace transform of Eq. 3.16 to get

$$D_S \left. \frac{\partial \bar{X}}{\partial r} \right|_{r=r_0} = K_f(\bar{Y} - \bar{Y}_{int}) \quad (3.31)$$

Where each member of Eq. 3.31 is a function of z only.

Take Laplace transform of Eq. 3.7 to get

$$\bar{Y}_{int} = K\bar{X}(r_0) \quad (3.32)$$

Evaluate Eq. 3.28 at $r=r_0$ and combine it with Eq. 3.32 to get

$$\bar{Y}_{int} = C_1 K r_0^{-1/2} I_{1/2}\left(\sqrt{\frac{S}{D_S}} r_0\right) \quad (3.33)$$

Substitute Eqs. 3.29 and 3.33 into Eq. 3.31

$$C_1 D_S \sqrt{\frac{S}{D_S}} \cdot r_o^{-1/2} I_{3/2}(\sqrt{\frac{S}{D_S}} r_o) = K_f \bar{Y} - c_1 K_f \cdot K r_o^{-1/2} I_{1/2}(\sqrt{\frac{S}{D_S}} r_o)$$

Therefore

$$C_1 = \frac{K_f \bar{Y}}{\sqrt{D_S S} \cdot r_o^{-1/2} \cdot I_{3/2}(\sqrt{\frac{S}{D_S}} r_o) + K_f K r_o^{-1/2} \cdot I_{1/2}(\sqrt{\frac{S}{D_S}} r_o)} \quad (3.34)$$

Combine Eqs. 3.33 and 3.34

$$\begin{aligned} \bar{Y}_{int} &= \frac{K_f K r_o^{-1/2} I_{1/2}(\sqrt{\frac{S}{D_S}} r_o) \bar{Y}}{\sqrt{D_S S} r_o^{-1/2} I_{3/2}(\sqrt{\frac{S}{D_S}} r_o) + K_f K r_o^{-1/2} I_{1/2}(\sqrt{\frac{S}{D_S}} r_o)} \\ &= \frac{K_f K I_{1/2}(\sqrt{\frac{S}{D_S}} r_o) \bar{Y}}{\sqrt{D_S S} I_{3/2}(\sqrt{\frac{S}{D_S}} r_o) + K_f K I_{1/2}(\sqrt{\frac{S}{D_S}} r_o)} \end{aligned} \quad (3.35)$$

Combine Eqs. 3.35 and 3.30 to obtain an ordinary differential equation in terms of \bar{Y}

$$\frac{d^2 \bar{Y}}{dz^2} - A \frac{d\bar{Y}}{dz} - (BS + D(S)) \bar{Y} = 0 \quad (3.36)$$

where

$$A = \left(\frac{v}{\epsilon E_D} \right)$$

$$B = \frac{1}{E_D}$$

$$D(S) = \frac{1 - \epsilon}{\epsilon} \cdot \frac{\alpha_f + 1}{E_D r_o} \cdot K_f \left(1 - \frac{K_f K I_{1/2}(\sqrt{\frac{S}{D_S}} r_o)}{\sqrt{D_S S} I_{3/2}(\sqrt{\frac{S}{D_S}} r_o) + K_f K I_{1/2}(\sqrt{\frac{S}{D_S}} r_o)} \right)$$

The solution of Eq. 3.36 is

$$(D - r_1)(D - r_2)Y = 0$$

$$r_1, r_2 = \frac{A \pm \sqrt{A^2 + 4(BS + D(S))}}{2}$$

Therefore

$$\bar{Y} = e^{\frac{A}{2}z} \left[C_3 \cdot \sinh \frac{\sqrt{A^2 + 4(BS + D(S))}}{2} z + C_4 \cosh \frac{\sqrt{A^2 + 4(BS + D(S))}}{2} z \right] \quad (3.37)$$

Since we are interested in the effluent concentration, the constants C_3 and C_4 should be evaluated using boundary conditions expressed by Eqs. 3.10 and 3.11. Neglecting the second member of Eq. 3.10, for constant y_{in} , the Laplace transform of Eq. 3.10

$$\text{is } \bar{Y}|_{z=0} = - \frac{(y_{in} - y_0)}{s}$$

Therefore from Eq. 3.37,

$$C_4 = - \frac{y_{in} - y_0}{s} \quad (3.38)$$

From Eq. 3.14,

$$\text{at } z = L, \frac{d^2y}{dz^2} = 0 \text{ or } \frac{d^2\bar{Y}}{dz^2} = 0$$

But from Eq. 3.36,

$$\frac{d^2\bar{Y}}{dz^2} = A \frac{d\bar{Y}}{dz} + (Bs + D(s))\bar{Y}$$

Therefore

$$A \frac{d\bar{Y}}{dz} \Big|_{z=L} + (Bs + D(s))\bar{Y} \Big|_{z=L} = 0$$

From Eq. 3.37,

$$\frac{d\bar{Y}}{dz} = \frac{A}{2} \exp\left(\frac{A}{2}z\right) \left[C_3 \cdot \sinh \frac{b}{2}z + C_4 \cdot \cosh \frac{b}{2}z \right]$$

$$+ \exp\left(\frac{A}{2}z\right) \left[C_3 \cdot \frac{b}{2} \cdot \cosh \frac{b}{2}z + C_4 \cdot \frac{b}{2} \cdot \sinh \frac{b}{2}z \right]$$

Therefore

$$\begin{aligned}
& \frac{A^2}{2} \exp\left(\frac{A}{2}L\right) \left[C_3 \cdot \sinh \frac{b}{2}L + C_4 \cdot \cosh \frac{b}{2}L \right] \\
& + A \exp\left(\frac{A}{2}L\right) \left[C_3 \frac{b}{2} \cosh \frac{b}{2}L + C_4 \frac{b}{2} \sinh \frac{b}{2}L \right] \\
& + (Bs + D(s)) \cdot \exp\left(\frac{A}{2}L\right) \left[C_3 \sinh \frac{b}{2}L + C_4 \cosh \frac{b}{2}L \right] = 0 \\
C_3 = & - \frac{\frac{A^2}{2} \cosh \frac{b}{2}L + A \frac{b}{2} \sinh \frac{b}{2}L + (Bs + D(s)) \cosh \frac{b}{2}L}{\frac{A^2}{2} \sinh \frac{b}{2}L + A \frac{b}{2} \cosh \frac{b}{2}L + (Bs + D(s)) \sinh \frac{b}{2}L} \cdot C_4 \quad (3.39)
\end{aligned}$$

where

$$b = \sqrt{A^2 + 4(Bs + D(s))}$$

$$\sinh u = u + \frac{u^3}{3!} + \frac{u^5}{5!} + \frac{u^7}{7!} + \dots \quad (3.40)$$

$$\cosh u = 1 + \frac{u^2}{2!} + \frac{u^4}{4!} + \frac{u^6}{6!} + \dots \quad (3.41)$$

$$I_{1/2}(u) = \sum_{k=0}^{\infty} \frac{\left(\frac{u}{2}\right)^{2k+1/2}}{k!(k+1/2)!} = \frac{\left(\frac{u}{2}\right)^{1/2}}{\frac{1}{2}!} + \frac{\left(\frac{u}{2}\right)^{5/2}}{\left(1\frac{1}{2}\right)!} + \frac{\left(\frac{u}{2}\right)^{9/2}}{2!(2\frac{1}{2})!!} + \dots$$

$$I_{3/2}(u) = \sum_{k=0}^{\infty} \frac{\left(\frac{u}{2}\right)^{2k+3/2}}{k!(k+3/2)!} = \frac{\left(\frac{u}{2}\right)^{3/2}}{\left(\frac{3}{2}\right)!} + \frac{\left(\frac{u}{2}\right)^{7/2}}{\left(\frac{5}{2}\right)!} + \frac{\left(\frac{u}{2}\right)^{11/2}}{2!(\frac{7}{2})!} + \dots$$

To invert Eq. 3.37 to time domain, an understanding of the method of residues is paramount to the effective inversion of the Laplace transformation. If,

$$\bar{f}(s) = \frac{p(s)}{q(s)}$$

where $p(s)$ and $q(s)$ are analytic at s_n (polynomials of s) and $q(s_n) = 0$ while $q'(s_n) \neq 0$ and $p(s_n) \neq 0$, then the residue of $f(s)$ at pole s_n is

$$p_n(t) = \frac{p(s_n)}{q'(s_n)} \exp(s_n t) \text{ for simple pole}$$

where

$$q'(s_n) = \left. \frac{dq(s)}{ds} \right|_{s=s_n}$$

Then

$$f(t) = L^{-1} \left\{ \frac{p(s)}{q(s)} \right\} = \sum_{n=1}^{\infty} \rho_n(t)$$

For the problem at hand,

$$\bar{Y} = \exp\left(\frac{A}{2}z\right) [C_3 \sinh \frac{b}{2}z + C_4 \cosh \frac{b}{2}z] \quad (3.37)$$

and combining Eqs. 3.38 and 3.39,

$$C_3 = \frac{y_{in} - y_0}{s} \cdot \frac{\frac{A^2}{2} \cosh \frac{b}{2}L + \frac{Ab}{2} \sinh \frac{b}{2}L + (Bs + D(s)) \cosh \frac{b}{2}L}{\frac{A^2}{2} \sinh \frac{b}{2}L + \frac{Ab}{2} \cosh \frac{b}{2}L + (Bs + D(s)) \sinh \frac{b}{2}L} \quad (3.42)$$

Check to ascertain that all terms are polynomial of s

$$I_{1/2}(\alpha s^{1/2}) = a_1 s^{1/4} + a_2 s^{1+1/4} + a_3 s^{2+1/4} + \dots = \frac{r_0^{1/2}}{2^{1/2} \cdot \frac{1}{2}! D_S^{1/4}} s^{1/4} + \dots$$

with $\alpha \equiv r_0/D_S^{1/2}$

$$I_{3/2}(\alpha s^{1/2}) = b_1 s^{3/4} + b_2 s^{1+3/4} + b_3 s^{2+3/4} + \dots = \frac{r_0^{3/2} s^{3/4}}{2^{3/2} \cdot (\frac{3}{2})! D_S^{3/4}} + \dots$$

$$s^{1/2} I_{3/2}(\alpha s^{1/2}) = b_1 s^{1+1/4} + b_2 s^{2+1/4} + b_3 s^{3+1/4} + \dots = \frac{r_0^{3/2} s^{1+1/4}}{2^{3/2} \cdot (\frac{3}{2})! D_S^{3/4}} + \dots$$

Therefore

$$\frac{I_{1/2}(s^{1/2})}{s^{1/2} I_{3/2}(s^{1/2}) + I_{1/2}(s^{1/2})} = \text{function of polynomial of } s = C_0 + C_1 s + C_2 s^2 + \dots$$

This also means that

$$D(s) = \text{polynomial of } s$$

Therefore

$$\frac{b}{2}L = \frac{A^2 + 4(Bs + D(s))}{2}L = \sqrt{\text{polynomial of } s} = d_0 + d_1s + d_2s^2 + \dots$$

From Eq. 3.41,

$$\cosh \frac{b}{2}L = \text{function of polynomial of } s = e_0 + e_1s + e_2s^2 + \dots$$

and from Eq. 3.40,

$$\left(\frac{b}{2}L\right)^{-1} \cdot \sinh \frac{b}{2}L = \text{function of polynomial of } s = f_0 + f_1s + f_2s^2 + \dots$$

In order to have Eq. 3.37 in the form of

$$\bar{Y} = \frac{p(s)}{q(s)} = \frac{(\text{polynomial of } s)_1}{(\text{polynomial of } s)_2} ,$$

Equation 3.42 must be multiplied by $(b/2) \cdot L$ in the numerator and denominator. Therefore

$$\bar{Y} = \exp\left(\frac{A}{2}z\right) \left[-\frac{p_1(s)}{q_1(s)} + \frac{p_2(s)}{q_2(s)} \right] \quad (3.43)$$

where

$$p_1(s) = (y_{in} - y_0) \cosh \frac{b}{2}z$$

$$q_1(s) = s$$

$$p_2(s) = (y_{in} - y_0) \left[\frac{A^2}{2} + A \frac{b}{2} \tanh \frac{b}{2}L + (Bs + D(s)) \right] \frac{\sinh \frac{b}{2}z}{\frac{b}{2}L}$$

$$q_2(s) = s \left[\frac{A^2}{2} \frac{\tanh \frac{b}{2}L}{\frac{b}{2}L} + \frac{A}{L} + (Bs + D(s)) \frac{\tanh \frac{b}{2}L}{\frac{b}{2}L} \right]$$

poles of $\frac{p_1(s)}{q_1(s)}$ at $s = 0$

Therefore the residue $\rho(t) = \frac{p_1(s=0)}{q_1'(s=0)} \exp(0 \cdot t)$

$$q_1'(s) = 1$$

$$\begin{aligned} p(s=0) &= (y_{in} - y_0) \cdot \cosh \frac{\sqrt{A^2 + 4D(s=0)}}{2} z \\ &= (y_{in} - y_0) \cdot \cosh \frac{A}{2} z \end{aligned}$$

Poles of $\frac{p_2(s)}{q_2(s)}$ at $s_1 = 0$ and s_n , $n = 2, 3, 4, \dots$

$$q_2(s_n) = 0$$

$$s_n \left\{ \frac{A^2 \tanh \frac{b}{2} L}{\frac{b}{2} L} + \frac{A}{L} + (Bs_n + D(s_n)) \frac{\tanh \frac{b}{2} L}{\frac{b}{2} L} \right\} = 0$$

$$s_1 = 0 \text{ first pole of } \frac{p_2(s)}{q_2(s)}; \rho_1 = \frac{p_2(s_1=0)}{q_2'(s_1=0)} \cdot 1$$

also

$$\frac{A^2 \tanh \frac{b}{2} L}{\frac{b}{2} L} + \frac{A}{L} + (Bs_n + D(s_n)) \frac{\tanh \frac{b}{2} L}{\frac{b}{2} L} = 0 \quad (3.44)$$

$$n = 2, 3, 4, \dots$$

Let

$$\frac{b}{2} L \Big|_{s=s_n} = i\lambda_n \quad (3.45)$$

then

$$\tanh \frac{b}{2} L = \tanh i\lambda_n = i \tan \lambda_n \quad (3.46)$$

also

$$\sqrt{A^2 + 4(Bs_n + D(s_n))} = i\lambda_n \cdot \frac{2}{L}$$

$$\begin{aligned}
\sqrt{A^2 + 4(Bs_n + D(s_n))} &= \frac{4\lambda_n^2}{L} \\
(Bs_n + D(s_n)) &= -\frac{\frac{4\lambda_n^2}{L} - A^2}{4} \\
&= -\frac{\lambda_n^2}{L} - \frac{A^2}{4}
\end{aligned} \tag{3.47}$$

Equation 3.44 becomes

$$\frac{A^2}{2} \cdot \frac{i \tan \lambda_n}{i \lambda_n} + \frac{A}{L} - \left(\frac{\lambda_n^2}{L} + \frac{A^2}{4} \right) \cdot \frac{i \tan \lambda_n}{i \lambda_n} = 0$$

or

$$\begin{aligned}
\tan \lambda_n &= \frac{\frac{A}{L} \cdot \lambda_n}{\frac{\lambda_n^2}{L} - \frac{A^2}{4}} \\
&= \frac{4A\lambda_n}{4\lambda_n^2 - LA^2}
\end{aligned} \tag{3.48}$$

Solve for λ_n , $n = 2, 3, 4, \dots$

Eq. 3.48 is a transcendental equation and the roots λ_n must be solved graphically or by computer. Numerically if $LA^2/4 = L/4(v/E_D)^2$ is large, it means that the diffusivity of the molecules are small (for molecules with very large molecular weight). In this case, one would have the special case of Figure 3.3. Knowing values of λ_n from Eq. 3.48, values of s_n , $n = 2, 3, 4, \dots$ can be calculated numerically from Eq. 3.47. Since $Y(z,t)$ decreases with t , s_n , $n = 2, 3, 4, \dots$ should be negative quantities.

Now find

$$q_2'(s_n) = \left. \frac{dq_2(s)}{ds} \right|_{s=s_n}$$

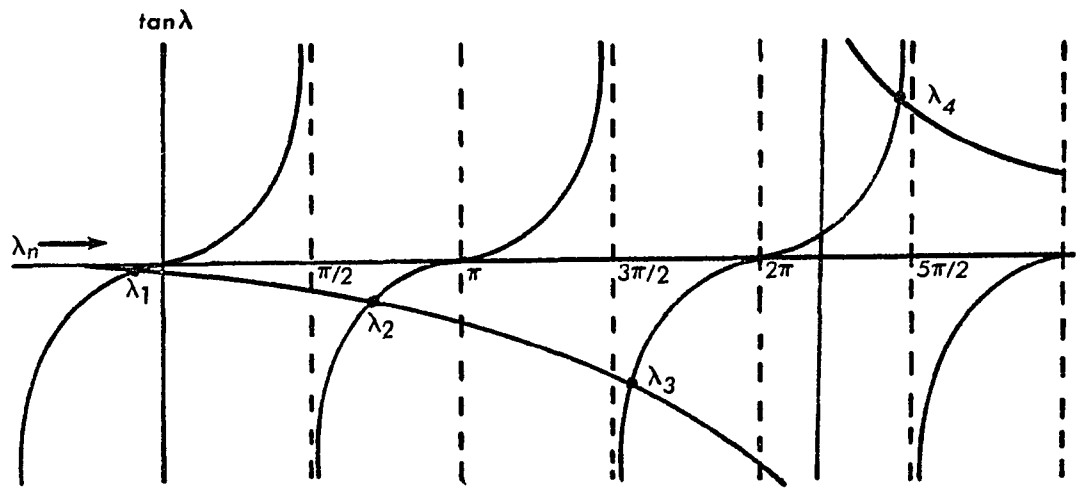


FIGURE 3.2 ROOTS OF $\tan \lambda_n = \lambda_n$

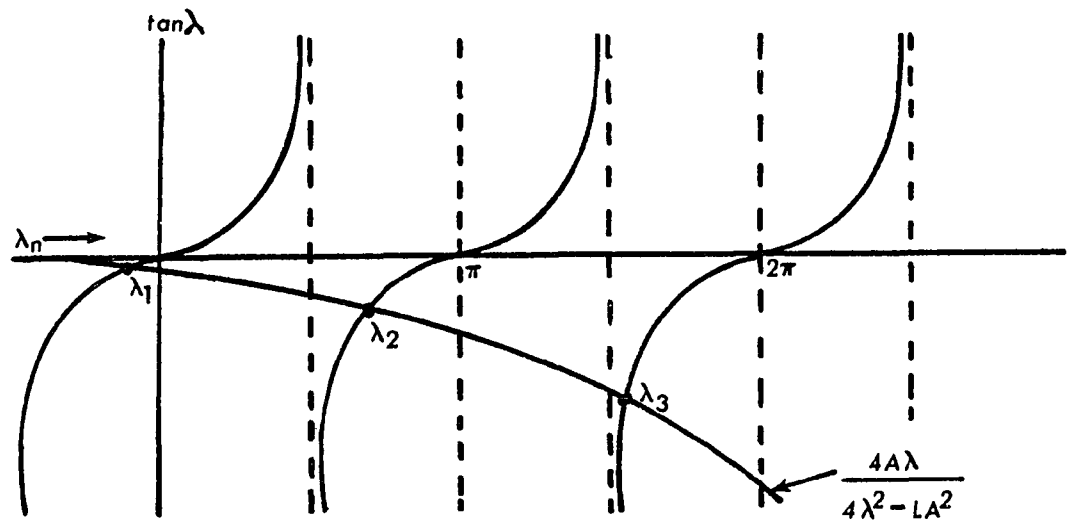


FIGURE 3.3 ROOTS OF $f(\lambda_n)$ WHEN $\frac{LA^2}{4} \rightarrow \infty$

$$\frac{d}{dx}[xI_p(\alpha x)] = \alpha x^p I_{p-1}(\alpha x)$$

$$\frac{d}{dx}[I_p(\alpha x)] = \alpha I_{p-1}(\alpha x) - \frac{p}{x} I_p(\alpha x)$$

$$D(s) = K_{f_0} \left[1 - \frac{K_f K I_{1/2}(\sqrt{s/D_S} r_0)}{D_S s I_{3/2}(\sqrt{s/D_S} r_0) + K_f K I_{1/2}(\sqrt{s/D_S} r_0)} \right]$$

where

$$K_{f_0} = \frac{1 - \epsilon}{\epsilon} \cdot \frac{\alpha_f + 1}{E d r_0} \cdot K_f$$

$$\frac{dD(s)}{ds} = \frac{K_f K (r_0/2\sqrt{D_S s} \cdot I_{3/2}(\sqrt{s/D_S} r_0) + 1/4s \cdot I_{1/2}(\sqrt{s/D_S} r_0))}{\sqrt{D_S s} I_{3/2}(\sqrt{s/D_S} r_0) + K_f K I_{1/2}(\sqrt{s/D_S} r_0)}$$

$$+ \frac{K_f K I_{1/2}(\sqrt{s/D_S} r_0) \cdot [r_0/\sqrt{D_S} s^{3/4} I_{1/2}(\sqrt{s/D_S} r_0)]}{[\sqrt{s D_S} I_{3/2}(\sqrt{s/D_S} r_0) + K_f K I_{1/2}(\sqrt{s/D_S} r_0)]^2}$$

$$+ \frac{K_f K \{ r_0/2\sqrt{s D_S} I_{3/2}(\sqrt{s/D_S} r_0) + \frac{1}{4} s I_{1/2}(\sqrt{s/D_S} r_0) \}}{[\sqrt{s D_S} I_{3/2}(\sqrt{s/D_S} r_0) + K_f K I_{1/2}(\sqrt{s/D_S} r_0)]^2}$$

$$\equiv F(s)$$

$$b = \sqrt{A^2 + 4(Bs + D(s))}$$

$$\frac{d(\frac{b}{2}L)}{ds} = \frac{L}{2} \cdot \frac{1}{2} \cdot \frac{4B + 4 \frac{dD(s)}{ds}}{\sqrt{A^2 + 4(Bs + D(s))}}$$

$$= \frac{B + F(s)}{\sqrt{A^2 + 4(Bs + D(s))}} L$$

$$\equiv H(s)$$

$$\frac{d(\tanh \frac{b}{2}L)}{ds} = \frac{d(\tanh \frac{b}{2}L)}{d(\frac{b}{2}L)} \cdot \frac{d(\frac{b}{2}L)}{ds}$$

$$\begin{aligned}
& + (\operatorname{sech} \frac{b}{2L})^2 \cdot \frac{B + F(S)}{\sqrt{A^2 + 4(Bs + D(s))}} \cdot L \\
& = L(B + F(s)) \cdot \frac{[\operatorname{sech} \frac{b}{2L}]^2}{b} \\
& \equiv G(s)
\end{aligned}$$

Therefore,

$$\begin{aligned}
q_2(s) & = s \left[\frac{A^2}{2} \frac{\tanh \frac{b}{2L}}{\frac{b}{2L}} + \frac{A}{L} + (Bs + D(s)) \frac{\tanh \frac{b}{2L}}{\frac{b}{2L}} \right] \\
q_2^1(s) & = \frac{A^2}{2} \frac{\tanh \frac{b}{2L}}{\frac{b}{2L}} + \frac{A}{L} + (Bs + D(s)) \frac{\tanh \frac{b}{2L}}{\frac{b}{2L}} \\
& + s \left\{ \frac{A^2}{2} \left[\frac{G(s)}{\frac{b}{2L}} - \frac{(\tanh \frac{b}{2L}) \cdot H(s)}{(\frac{b}{2L})^2} \right] + (B + F(s)) \frac{\tanh \frac{b}{2L}}{\frac{b}{2L}} \right. \\
& \left. + \frac{Bs + D(s)}{\frac{b}{2L}} \cdot G(s) - \frac{(Bs + D(s))}{(\frac{b}{2L})^2} \cdot \tanh \frac{b}{2L} \cdot H(s) \right\}
\end{aligned}$$

The final solution is

$$Y(z, t) = \exp\left(\frac{A}{2}z\right) \left[-L^{-1} \left\{ \frac{p_1(s)}{q_1(s)} \right\} + L^{-1} \left\{ \frac{p_2(s)}{q_2(s)} \right\} \right]$$

$$\begin{aligned}
Y(z, t) & = \exp\left(\frac{A}{2}z\right) \left[-(y_{in} - y_0) \cdot \cosh \frac{A}{2}z + \frac{p_2(s_1=0)}{q_1^1(s_1=0)} + \sum_{n=2}^{\infty} \frac{p_2(s_n)}{q_1^1(s_n)} \exp(s_n t) \right] \\
& \qquad \qquad \qquad (3.49)
\end{aligned}$$

SIMPLIFIED MODEL--NO AXIAL DISPERSION

For the fixed bed adsorption shown in Figure 3.1, only concentration gradients in the axial direction caused by the

bulk flow are considered. All radial gradients, axial dispersion and the like are ignored. The material balance for both fluid and solid is as follows:

$$\text{Liquid: } \frac{\partial y}{\partial t} + \frac{v}{\epsilon} \frac{\partial y}{\partial z} = -\lambda(y - y^*) \quad (3.50)$$

$$\text{Solid: } \frac{\partial x}{\partial t} = \left(\frac{\epsilon}{1 - \epsilon}\right)\lambda(y - y^*) \quad (3.51)$$

$$\lambda = \frac{k(T)a}{\epsilon} = \text{mass transfer coefficient, sec}^{-1}$$

Rewriting Eqs. 3.50 and 3.51, we get

$$\epsilon sc \frac{\partial y}{\partial t} + vsc \frac{\partial y}{\partial z} + (1 - \epsilon)cs \frac{\partial x}{\partial t} = 0 \quad (3.50a)$$

$$(1 - \epsilon)cs \frac{\partial x}{\partial t} = sk(T)a(y - y^*) \quad (3.51a)$$

By method of combination of variables, define

$$t' = t - z \left(\frac{\epsilon sc}{v}\right) \quad (3.52)$$

Since

$$y = y(z, t) = y(z, t')$$

$$\frac{\partial y}{\partial t} = \left(\frac{\partial y}{\partial t'}\right)_z \frac{\partial t'}{\partial t} + \left(\frac{\partial y}{\partial z}\right)_{t'} \frac{\partial z}{\partial t} \quad (3.53)$$

and

$$\frac{\partial y}{\partial z} = \left(\frac{\partial y}{\partial t'}\right)_z \frac{\partial t'}{\partial z} + \left(\frac{\partial y}{\partial z}\right)_{t'} \frac{\partial z}{\partial z}$$

Therefore

$$\frac{\partial y}{\partial z} = - \frac{\partial y}{\partial t'} \left(\frac{\epsilon sc}{csv}\right) + \frac{\partial y}{\partial z} \quad (3.54)$$

Substituting Eqs. 3.53 and 3.54 into Eq. 3.50a to get

$$\frac{\partial y}{\partial z} = - \frac{sk(T)a}{c_{sv}}(y - y^*) \quad (3.55)$$

Rewriting Eq. (3.51a) in terms of Eq. 3.52,

$$x = x(z, t)$$

$$\frac{\partial x}{\partial t'} = \left(\frac{\partial x}{\partial t'} \right)_z \cdot \left(\frac{\partial t'}{\partial t} \right)_z + \left(\frac{\partial x}{\partial z} \right)_{t'} \cdot \left(\frac{\partial z}{\partial t} \right)_z \quad (3.56)$$

Therefore Eq. 3.51a becomes

$$\frac{\partial x}{\partial t'} = \frac{k(T)a}{(1 - \epsilon)c} (y - y^*) \quad (3.57)$$

Assuming a linear equilibrium distribution,

$$y^* = mx \quad (3.58)$$

Equations 3.56-3.58 are solved based on the following boundary conditions:

$$\text{I.C.: at } t' = 0, x = 0 \quad \text{for all } z > 0 \quad (3.59)$$

$$\text{B.C.: at } z = 0, y = y_i \quad \text{for all } t' > 0 \quad (3.60)$$

Equations 3.56-3.58 are easily solvable when written in dimensionless variables.

Therefore,

$$\text{let } Y = \frac{y}{y_i} \quad (3.61)$$

$$X = \frac{mx}{y_i} \quad (3.62)$$

$$\zeta = \frac{zk(T)a}{vc} \quad (3.63)$$

$$\tau = \frac{mt'k(T)a}{(1 - \epsilon)c} \quad (3.64)$$

Substituting Eqs. 3.63-3.64 into Eqs. 3.55 and 3.57, we get

$$\frac{\partial Y}{\partial \zeta} = -(Y - X) \quad (3.65)$$

and

$$\frac{\partial X}{\partial \tau} = (Y - X) \quad (3.66)$$

and the boundary conditions become

$$\text{I.C.: at } \tau = 0, X = 0 \quad \text{for all } \zeta \quad (3.67)$$

$$\text{B.C.: at } \zeta = 0, Y = 1 \quad \text{for all } \tau \quad (3.68)$$

Laplace transform Eqs. 3.65 and 3.66 with respect to τ

$$\frac{d\bar{Y}}{d\zeta} = -\bar{Y} + \bar{X} \quad (3.69)$$

$$s\bar{X} = \bar{Y} - \bar{X} \quad \text{or} \quad \bar{X} = \frac{1}{s+1} \bar{Y} \quad (3.70)$$

Combine Eqs. 3.69 and 3.70

$$\frac{d\bar{Y}}{d\zeta} = -\bar{Y} + \frac{1}{s+1} \bar{Y} = -\frac{s}{s+1} \bar{Y} \quad (3.71)$$

Integrate Eq. 3.71 using Eq. 3.68 (B.C. 2)

$$\int_{\bar{Y}=\frac{1}{s}}^{\bar{Y}} \frac{d\bar{Y}}{\bar{Y}} = -\frac{s}{s+1} \int_{\zeta=0}^{\zeta} d\zeta \quad (3.72)$$

$$\ln \bar{Y} - \ln \frac{1}{s} = -\frac{s}{s+1} \zeta$$

$$s\bar{Y} = \exp\left(-\frac{s}{s+1} \zeta\right)$$

or

$$\bar{Y}(\zeta, \tau) = \frac{1}{s} \exp\left(-\frac{s}{s+1} \zeta\right) \quad (3.73)$$

and

$$\bar{X} = \frac{1}{s+1} \cdot \frac{1}{s} \cdot \exp\left(-\frac{s}{s+1} \zeta\right)$$

or

$$\bar{X}(\zeta, \tau) = \frac{1}{s} \cdot \frac{\exp\left(-\frac{s}{s+1} \zeta\right)}{s+1} \quad (3.74)$$

Take the inverse transform of Eq. 3.73

$$\begin{aligned}
Y(\zeta, \tau) &= \frac{1}{s} \cdot e^{-\frac{s}{s+1} \zeta} \\
&= \frac{1}{s} e^{-\frac{s+1-1}{s+1} \zeta} \\
&= \frac{1}{s} e^{-\zeta} e^{+\frac{\zeta}{s+1}} \\
&= e^{-\zeta} \left[\frac{s+1}{s} \cdot \frac{e^{\frac{\zeta}{s+1}}}{s+1} \right] \\
&= e^{-\zeta} \left[\left(1 + \frac{1}{s}\right) \cdot \frac{e^{\frac{\zeta}{s+1}}}{s+1} \right] \\
Y(\zeta, \tau) &= e^{-\zeta} \left[\frac{e^{\frac{\zeta}{s+1}}}{s+1} + \frac{1}{s} \cdot \frac{e^{\frac{\zeta}{s+1}}}{s+1} \right] \tag{3.75}
\end{aligned}$$

Equation 3.75 is now transformable by method of convolution.

<u>f(s)</u>	<u>F(t)</u>
$f(s-a)$	$e^{at} \cdot F(t)$
$\frac{1}{s} e^{-\frac{k}{s}}$	$J_0(2\sqrt{kt})$
$f_1(s) \cdot f_2(s)$	$F_1 * F_2 = \int_0^t F_1(t-\sigma) F_2(\sigma) d\sigma$
$\frac{1}{s+1} e^{\frac{\zeta}{s+1}}$	$e^{-\zeta} \cdot J_0(2\sqrt{-\zeta\tau})$
$\frac{1}{s+1} \frac{e^{\frac{\zeta}{s+1}}}{s+1}$	$\int_0^\tau 1 \cdot e^{-\sigma} \cdot J_0(2\sqrt{-\zeta\tau}) d\sigma$

Therefore Eq. 3.75 becomes

$$\begin{aligned}
Y(\zeta, \tau) &= L^{-1}[\bar{Y}] \\
&= e^{-\zeta} \left[e^{-\tau} J_0(i\sqrt{4\zeta\tau}) + \int_0^\tau e^{-\sigma} \cdot J_0(i\sqrt{4\zeta\sigma}) d\sigma \right] \\
Y(\zeta, \tau) &= e^{-(\zeta+\tau)} \cdot J_0(i\sqrt{4\zeta\tau}) + \int_0^\tau e^{-(\zeta+\sigma)} J_0(i\sqrt{4\zeta\sigma}) d\sigma \tag{3.76}
\end{aligned}$$

Using the same method of convolution, Eq. 3.74 can be transformed to

$$X(\zeta, \tau) = \int_0^{\tau} e^{-(\zeta + \sigma)} \cdot J_0(i\sqrt{4\zeta\sigma}) d\sigma \quad (3.77)$$

Equations 3.76 and 3.77 describe the fluid and solid phases concentration at any position and time space as an empty column is being saturated respectively at any desired temperature. Equations 3.76 and 3.77 represent an analytical solution when a step forcing function in concentration is imposed on the column as described by Eqs. 3.59 and 3.60. If a pulse forcing function in concentration is imposed on the column, the following initial and boundary conditions are necessary.

$$\text{Initial Condition: at } t' = 0, \text{ for } z > 0, \quad x = 0 \quad (3.78)$$

Equation 3.78 implies that the liquid phase concentration must be zero for $t'_0 > (z\epsilon s/v)$ (see Eq. 3.52), where t'_0 is the time duration for which the pulse is applied.

$$\begin{aligned} \text{Boundary Condition: at } z = 0, \text{ for } 0 \leq t' \leq t'_0 \quad y = y_i \\ t' > t'_0 \quad y = 0 \end{aligned} \quad (3.79)$$

where

$$t'_0 = t_0 - \left(\frac{z\epsilon s}{v}\right)$$

Change Eqs. 3.78 and 3.79 to dimensionless variable (see Eqs. 3.63 and 3.64), and obtain

$$\text{I.C. at } \tau = 0, \quad X = 0 \quad \text{for all } \zeta \quad (3.80)$$

$$\text{B.C. at } \zeta = 0, \quad Y = u(\tau) - u(\tau - \tau') \text{ for all } \tau > 0 \quad (3.81)$$

Equation 3.81 means that

$$Y = 1 \quad \text{for } 0 < \tau \leq \tau'$$

and

$$Y = 0 \quad \text{for } \tau > \tau'$$

where

$$\tau' = \frac{mt_0'k(T)a}{(1-\epsilon)c}$$

The Laplace transform of Eqs. 3.80 and 3.81 are, respectively

$$\tau = 0, \quad \bar{X} = 0 \quad (3.80a)$$

$$\zeta = 0, \quad \bar{Y} = \frac{1}{s}(1 - e^{-\tau's}) \quad (3.81a)$$

Integrating Eq. 3.71 using Eq. 3.81a,

$$\int_{\bar{Y}=\frac{1}{s}(1-e^{-\tau's})}^{\bar{Y}} \frac{d\bar{Y}}{\bar{Y}} = -\frac{s}{s+1} \int_{\zeta=0}^{\zeta} ds \quad (3.82)$$

$$\ln \frac{s\bar{Y}}{1 - e^{-\tau's}} = -\frac{s}{s+1} \zeta$$

$$s\bar{Y} = (1 - e^{-\tau's})e^{-\left(\frac{s}{s+1}\right)\zeta}$$

or

$$\bar{Y} = [1 - \exp(-\tau's)] \left[\frac{1}{s} \exp\left(-\frac{s}{s+1}\zeta\right) \right] \quad (3.83)$$

and

$$\bar{X} = \frac{1}{s+1} \bar{Y}$$

or

$$\bar{X} = [1 - \exp(-\tau's)] \left[\frac{1}{s(s+1)} \exp\left(-\frac{s}{s+1}\zeta\right) \right] \quad (3.84)$$

Take the inverse Laplace transform of Eqs. 3.83 and 3.84.

$$\begin{aligned}
\bar{Y} &= (1 - e^{-\tau' s}) \left\{ e^{-\zeta} \left[\frac{1}{s+1} e^{\frac{\zeta}{s+1}} + \frac{1}{s} \left(\frac{1}{s+1} e^{\frac{\zeta}{s+1}} \right) \right] \right\} \\
&= \left\{ e^{-\left[\frac{1}{s+1} e^{\frac{\zeta}{s+1}} + \frac{1}{s} \left(\frac{1}{s+1} e^{\frac{\zeta}{s+1}} \right) \right]} \right\} \\
&- e^{-\tau' s} \left\{ e^{-\zeta} \left[\frac{1}{s+1} e^{\frac{\zeta}{s+1}} + \frac{1}{s} \left(\frac{1}{s+1} e^{\frac{\zeta}{s+1}} \right) \right] \right\} \quad (3.85)
\end{aligned}$$

By method of convolution, as previously outlined, and by shifting theorem,

$$\text{if } f(s) = e^{-\alpha s} f(s), \text{ then } F(t) = u(t - \alpha) F(t - \alpha)$$

Therefore, Eq. 3.85 becomes

$$\begin{aligned}
Y(\tau, \zeta) &= \left\{ e^{-(\zeta + \tau)} J_0(i\sqrt{4\zeta\tau}) + \int_0^{\tau} e^{-(\zeta + \sigma)} J_0(i\sqrt{4\zeta\sigma}) d\sigma \right\} u(\tau) \\
&- e^{-(\zeta + \tau - \tau')} J_0(i\sqrt{4\zeta(\tau - \tau')}) + \int_0^{\tau - \tau'} e^{-(\zeta + \sigma - \tau')} J_0(i\sqrt{4\zeta(\sigma - \tau')}) d\sigma \} u(\tau - \tau') \quad (3.86)
\end{aligned}$$

Therefore, for $0 < \tau \leq \tau'$,

$$Y(\tau, \zeta) = e^{-(\zeta + \tau)} J_0(i\sqrt{4\zeta\tau}) + \int_0^{\tau} e^{-(\zeta + \sigma)} J_0(i\sqrt{4\zeta\sigma}) d\sigma \quad (3.87)$$

and for $\tau > \tau'$, Eq. 3.86 is applicable.

Equation 3.84 becomes,

$$\begin{aligned}
\bar{X} &= (1 - e^{-\tau' s}) \left[e^{-\zeta} \left(\frac{1}{s} \left(\frac{1}{s+1} \right) e^{\frac{\zeta}{s+1}} \right) \right] \\
&= e^{-\zeta} \left[\frac{1}{s} \left(\frac{1}{s+1} \right) e^{\frac{\zeta}{s+1}} \right] - e^{-\tau' s} \left\{ e^{-\zeta} \left[\frac{1}{s} \left(\frac{1}{s+1} \right) e^{\frac{\zeta}{s+1}} \right] \right\} \quad (3.88)
\end{aligned}$$

Therefore

$$\begin{aligned}
 X(\tau, \zeta) = & \left\{ \int_0^{\tau} e^{-(\zeta+\sigma)} J_0(i\sqrt{4\zeta\sigma}) d\sigma \right\} u(\tau) - \\
 & \left\{ \int_0^{\tau} e^{-(\zeta+\sigma-\tau')} J_0(i\sqrt{4\zeta(\sigma-\tau')}) d\sigma \right\} u(\tau-\tau')
 \end{aligned} \tag{3.89}$$

for $0 < \tau \leq \tau'$,

$$X(\tau, \zeta) = \int_0^{\tau} e^{-(\zeta+\sigma)} J_0(i\sqrt{4\zeta\sigma}) d\sigma \tag{3.90}$$

and for $\tau > \tau'$, Eq. 3.89 is applicable.

CHAPTER 4
NUMERICAL SOLUTION

FINITE DIFFERENCE METHOD OF SOLUTION

An alternative method of solving the mass transport equation is by finite difference method. This method is particularly useful for solving higher order ordinary differential equations of boundary value types. The material balance under consideration in this section is a combination of Eqs. 3.50 and 3.51 to give

$$\epsilon \frac{\partial y}{\partial t} + (1 - \epsilon) \frac{\partial x}{\partial t} + v \frac{\partial y}{\partial z} = 0 \quad (4.1)$$

To begin the analysis of Eq. 4.1, let us consider the first-order differential equation,

$$\frac{dy}{dz} = f(z,y) \quad (4.2)$$

Each member of Eq. 4.1 is assumed to be continuous. In Eq. 4.2, if dy/dz is replaced by $y_i - y_{i-1} / z_i - z_{i-1}$, a difference equation of the first order is obtained,

$$\frac{y_i - y_{i-1}}{z_i - z_{i-1}} = f(z_i, y_i) \quad (4.3)$$

Upon rearrangement and evaluation over a time step j , Eq. 4.3 becomes

$$y(i,j) = y(i-1,j-1) + f[z(i,j-1), y(i,j-1)] \cdot [z(i,j-1) - z(i-1,j-1)] \quad (4.4)$$

In general, difference equations do not require even spacing

of the pivotal points, but assuming that Eq. 4.4 has an evenly spaced pivot, $z(i,j-1)-z(i-1,j-1)$ is replaced by Δz and we get

$$y(i,j-1) = y(i-1,j-1) + \Delta z f[z(i,j-1), y(i,j-1)] \quad (4.5)$$

Rearrange Eq. 4.5 to get

$$\frac{dy}{dz} = \frac{y(i,j-1) - y(i-1,j-1)}{\Delta z} = f[z(i,j-1), y(i,j-1)] \quad (4.6)$$

Similarly, other members of Eq. 4.1 can be written in finite difference form.

$$\frac{dy}{dt} = \frac{y(i,j) - y(i,j-1)}{\Delta t} \quad (4.7)$$

$$\frac{dx}{dt} = \frac{x(i,j) - x(i,j-1)}{\Delta t} \quad (4.8)$$

Substituting Eqs. 4.6 through 4.8 into Eq. 4.1, we get

$$\epsilon \left[\frac{y(i,j) - y(i,j-1)}{\Delta t} \right] + (1-\epsilon) \left[\frac{x(i,j) - x(i,j-1)}{\Delta t} \right] + \frac{q}{s} \left[\frac{y(i,j-1) - y(i-1,j-1)}{\Delta z} \right] = 0 \quad (4.9)$$

where $v = q/s$

Multiply Eq. 4.9 by Δt and $s\Delta z$,

$$v[y(i,j) - y(i,j-1)] + \bar{V}[x(i,j) - x(i,j-1)] + V[y(i,j-1) - y(i-1,j-1)] = 0 \quad (4.10)$$

where

$V = \epsilon s \Delta z = q \Delta t =$ volume of solute in the fluid phase

$\bar{V} = (1-\epsilon) s \Delta z =$ volume of solute in the solid phase

$s =$ cross sectional area of empty column

Rearranging Eq. 4.10, we obtain

$$V y(i, j) - V y(i, j-1) + \bar{V} x(i, j) - \bar{V} x(i, j-1) = V y(i-1, j-1) - V y(i, j-1)$$

or

$$V y(i, j) + \bar{V} x(i, j) = V y(i-1, j-1) + \bar{V} x(i, j-1) \quad (4.11)$$

Let

$$x = K(T)y \quad (4.12)$$

= linear equilibrium relation for the solute
between solid and liquid phases

Expressing the equilibrium relation in finite difference form, we get

$$x(i, j-1) = K(i, j-1)y(i, j-1) \quad (4.13)$$

and

$$x(i, j) = K(i, j)y(i, j) \quad (4.14)$$

Substitute Eqs. 4.13 and 4.14 into Eq. 4.11

$$V y(i, j) + \bar{V} K(i, j)y(i, j) = V y(i-1, j-1) + \bar{V} K(i, j-1)y(i, j-1)$$

or

$$y(i, j)[V + \bar{V} K(i, j)] = V y(i-1, j-1) + \bar{V} K(i, j-1)y(i, j-1) \quad (4.15)$$

Upon rearrangement,

$$y(i, j) = \frac{V y(i-1, j-1) + \bar{V} K(i, j-1)y(i, j-1)}{V + \bar{V} K(i, j)} \quad (4.16)$$

Equation 4.16 is so general that it can be applied to calculate the concentration transients (Kerobo, 1979) for batch, continuous parapump and cyclic adsorption process simulation. The inputs of the computer simulation depends on the desired process, viz: batch or continuous, as the case may be,

but for cyclic adsorption process, a different algorithm is needed. The standard FORTRAN IV language was used for the simulation.

As can be readily seen from Eq. 4.16, the concentration for the next transfer step can be solved in terms of the concentrations in the previous transfer step. Since the linear isotherm constant, $K(T)$, is a function of temperature, and temperature varies with the time (j) step, it then becomes necessary to use the appropriate $K(T)$ value that corresponds to the temperature of the time step under consideration. The equilibrium isotherm shifts with temperature variation; therefore, the fluid mixture in the column and therefore the solute is expected to experience a change in concentration. Usually, the solute concentration in the fluid phase increases with an increase in temperature. At low temperature, the solute wave moves slowly and is held up by the stationary (solid) phase. A subsequent increase in the solute movement is attained as a step change in temperature is selectively imposed on the column.

In the computation of the concentration transients, it is assumed that local equilibrium between the liquid and the sorbent in the layers of the separating medium in the column is attained. Deviations from local equilibrium can be accounted for by introducing the concept of "effective plates" or "cells." In this discontinuous model, the fluid mixture in an effective plate of the bed attains equilibrium with the sorbent before it moves on into the next plate. The effluent thus consists of a

sequence of finite volumes of the fluid mixture, each of which is so large as to fill an effective plate. On their way through the column, these volumes are subjected to a series of equilibrations, one in each effective plate.

The assumption of equilibrium theory is particularly useful in simplifying the material balance made on the extensive variables of the column. The assumption of discrete (effective plate or cells) transfer equilibrium stage model was used by Jenczewski and Meyer (1970); Wankat (1974); Grevillot and Tondeur (1976); Kerobo (1979); and Chen et al. (1980a, 1980b, 1981). Although the equilibrium theory does overpredict the concentration transients, it enables us to have a clear insight of the parametric pumping process. For the system under investigation, the results of the breakthrough data exhibit a favorable (Langmuir type) adsorption isotherm. This phenomenon is indicative of competitive non-interactive adsorption by the adsorbates on the adsorbent sites. The breakthrough data were fitted to a modified Langmuir isotherm (Sweed, 1969) of the form

$$x_i = \frac{A y^*_{i}}{1 + B y^*_{i}} + D y^*_{i} \quad (4.17)$$

Therefore, to adequately simulate the concentration profiles of the effluent using the local equilibrium theory, the solid phase concentration must be calculated using Eq. 4.17 instead of Eq. 4.12. In the finite difference form, Eq. 4.17 becomes

$$x(I,J) = \frac{A y(I,J)}{1 + B y(I,J)} + D y(I,J) \quad (4.18a,b)$$

and

$$x(I, J-1) = \frac{Ay(I, J-1)}{1 + By(I, J-1)} + Dy(I, J-1)$$

The constants, A and B, in Eq. 4.17 or 4.18a,b are temperature dependent, while the constant, D, is a function of the adsorbate type. The equations necessary for calculating the concentration profiles by successive iterations are Eqs. 4.11 and 4.18.

Chen et al. (1981) predicted open parametric pumping by finite mass transfer, and a linear equilibrium adsorption was assumed (for dilute solution). In their work, the difference equations necessary for calculating the concentration transients as shown in their paper (Eqs. 7 and 9) are as follows:

$$y(I, J) = y(I-1, J-1) - \left(\frac{1-\epsilon}{\epsilon}\right)[x(I, J) - x(I, J-1)] \quad (7)$$

$$x(I, J) = \frac{y(I-1, J-1) + \left(\frac{1-\epsilon}{\epsilon}\right)x(I, J-1)}{\left(\frac{1-\epsilon}{\epsilon}\right) + \frac{1}{k}} + [x(I, J-1) - \frac{y(I-1, J-1) + \left(\frac{1-\epsilon}{\epsilon}\right)x(I, J-1)}{\left(\frac{1-\epsilon}{\epsilon}\right) + \frac{1}{k}}] \cdot \text{Exp}[-\lambda \left(\left(\frac{1-\epsilon}{\epsilon}\right) + \frac{1}{k}\right)\Delta t] \quad (9)$$

The development of the equations necessary for calculating $x(I, J)$ and $y(I, J)$ with non-linear adsorption isotherm is quite involved, as will be shown in the on-going analysis.

FINITE DIFFERENCE EQUATIONS FOR FINITE MASS TRANSFER WITH NON-LINEAR ADSORPTION ISOTHERM

For favorable adsorption isotherms of the Langmuir type, the solute material balances reflecting the events occurring within the adsorption column are

$$\epsilon v \frac{\partial y}{\partial z} + \epsilon \frac{\partial y}{\partial t} = -(1 - \epsilon) \frac{\partial x}{\partial t} \quad (4.19)$$

$$\frac{\partial x}{\partial t} = \lambda (y - y^*) \quad (4.20)$$

$$x = \frac{Ay^*}{1 + By^*} + Dy^* \quad (4.21)$$

Note that the asterisk, as shown in Eq. 4.21, indicates equilibrium with the solid (adsorbent) phase and it was omitted from Eqs. 4.17 and 4.18a,b when local equilibrium is assumed.

In writing Eqs. 4.19 through 4.21, plug flow was assumed, axial diffusion was neglected and the mass transfer coefficient λ is assumed to be only dependent on temperature. To obtain an equation analogous to Chen et al. (1981), but with non-linear adsorption isotherm of the Langmuir type, it is necessary to write Eqs. 4.19 through 4.21 in finite difference form to obtain an expression for y^* from Eq. 4.21 as a function of x and the physical constants.

$$x = \frac{1}{\frac{1}{Ay^*} + \frac{B}{A}} + \frac{D}{y^*}$$

or

$$x = \frac{1}{\bar{A}\bar{y} + C} + \frac{D}{\bar{y}}$$

where

$$\bar{A} = \frac{1}{A}, \quad \bar{y} = \frac{1}{y^*} \quad \text{and} \quad C = \frac{B}{A}$$

$$(x\bar{y} - D)(\bar{A}\bar{y} + C) = \bar{y}$$

$$\bar{A}_x \bar{y}^2 + (C_x - D\bar{A})\bar{y} - CD = \bar{y}$$

$$\bar{A}_x \bar{y}^2 + (C_x - D\bar{A} - 1)\bar{y} - CD = 0 \quad (4.22)$$

Equation 4.22 is in a quadratic form in y , and roots can be obtained by a quadratic formula.

$$\bar{y}_1, \bar{y}_2 = - \frac{(C_x - D\bar{A} - 1) \pm \sqrt{(C_x - D\bar{A} - 1)^2 + 4\bar{A}_x CD}}{2\bar{A}_x} \quad (4.23)$$

Equation 4.23 can be simplified greatly if the adsorbate type physical constant D is allowed to approach zero ($D \rightarrow 0$), in which case the two roots will be identical, viz:

$$\bar{y}_1, \bar{y}_2 = \frac{1 - C_x}{\bar{A}_x}$$

or

$$y^* = \frac{A^{-1}x}{1 - BA^{-1}x} \quad (4.24)$$

Replace the time and position derivatives in Eq. 4.19 by the lowest order backward differences:

$$\begin{aligned} & \epsilon v \Delta t [y(I, J-1) - y(I-1, J-1)] + \epsilon \Delta z [y(I, J) - y(I, J-1)] \\ & = -(1 - \epsilon) \Delta z [x(I, J) - x(I, J-1)] \end{aligned} \quad (4.25)$$

If

$\frac{H}{NZ} = \Delta z = v \Delta t$, where H = height of the column and NZ = position increments, then Eq. 4.25 now becomes,

$$y(I, J) = y(I-1, J-1) - \left(\frac{1 - \epsilon}{\epsilon}\right) [x(I, J) - x(I, J-1)] \quad (4.26)$$

Substitute Eqs. 4.24 and 4.26 into Eq. 4.20 to obtain

$$\frac{\partial x}{\partial t} = \lambda \left[y(I-1, J-1) - \left(\frac{1-\epsilon}{\epsilon}\right)x(I, J) + \left(\frac{1-\epsilon}{\epsilon}\right)x(I, J-1) - \frac{A^{-1}x(I, J)}{1-BA^{-1}x(I, J)} \right] \quad (4.27)$$

$$\begin{aligned} \text{Let } a &= y(I-1, J-1) + \left(\frac{1-\epsilon}{\epsilon}\right)x(I, J-1) \\ b &= -A^{-1} \\ c &= -BA^{-1} \\ f &= -\left(\frac{1-\epsilon}{\epsilon}\right) \end{aligned} \quad (4.28)$$

Equation 4.27 now becomes,

$$\begin{aligned} \frac{\partial x}{\partial t} &= \lambda \left[a + fx(I, J) + \frac{bx(I, J)}{1 + cx(I, J)} \right] \\ &= \lambda \left\{ \frac{a[1 + cx(I, J)] + fx(I, J)[1 + cx(I, J)] + bx(I, J)}{1 + cx(I, J)} \right\} \\ &= \lambda \left\{ \frac{a + acx(I, J) + fx(I, J) + cfx(I, J)^2 + bx(I, J)}{1 + cx(I, J)} \right\} \\ &= \lambda \left\{ \frac{cfx(I, J)^2 + (ac + b + f)x(I, J) + a}{1 + cx(I, J)} \right\} \\ &= \lambda \, cf \left\{ \frac{x(I, J)^2 + gx(I, J) + h}{1 + cx(I, J)} \right\} \end{aligned} \quad (4.29)$$

where

$$\begin{aligned} g &= \frac{ac + b + f}{cf} \\ h &= \frac{a}{cf} \end{aligned}$$

Upon rearrangement, Eq. 4.28 becomes

$$\frac{[1 + cx(I, J)]dx(I, J)}{x(I, J)^2 + gx(I, J) + h} = \lambda cfdt \quad (4.30)$$

To integrate Eq. 4.29, the left member has to be rearranged into two parts. Thus,

$$\frac{cx(I,J)dx(I,J)}{x(I,J)^2 + gx(I,J) + h} + \frac{dx(I,J)}{x(I,J)^2 + gx(I,J) + h} = \lambda cfdt \quad (4.29a)$$

Equation 4.30 can easily be integrated by using the following identities:

$$\int \frac{dx}{ax^2+bx+c} = \left\{ \begin{array}{l} \frac{2}{\sqrt{4ac-b^2}} \tan^{-1} \frac{2ax+b}{\sqrt{4ab-b^2}} \\ \frac{1}{b^2-4ac} \ln \left(\frac{2ax + b - \sqrt{b^2 - 4ac}}{2ax + b + \sqrt{b^2 - 4ac}} \right) \end{array} \right.$$

and

$$\int \frac{xdx}{ax^2 + bx + c} = \frac{1}{2a} \ln(ax^2 + bx + c) - \frac{b}{2a} \int \frac{dx}{ax^2 + bx + c}$$

Upon integration of Eq. 4.30 with respect to t over the time increment Δt ,

$$\begin{aligned} & \frac{c}{2} \ln[x(I,J)^2 + gx(I,J) + h] - \frac{gc}{2} \left\{ \frac{1}{\sqrt{g^2 - 4h}} \ln \left(\frac{2x(I,J) + g - \sqrt{g^2 - 4h}}{2x(I,J) + g + \sqrt{g^2 - 4h}} \right) \right\} \\ & + \frac{1}{\sqrt{g^2 - 4h}} \ln \left(\frac{2x(I,J) + g - \sqrt{g^2 - 4h}}{2x(I,J) + g + \sqrt{g^2 - 4h}} \right) = \lambda cf\Delta t \quad (4.30a) \end{aligned}$$

$$\begin{aligned} & \frac{c}{2} \ln[x(I,J)^2 + gx(I,J) + h] + \left(1 - \frac{gc}{2}\right) \frac{1}{\sqrt{g^2 - 4h}} \ln \left(\frac{2x(I,J) + g - \sqrt{g^2 - 4h}}{2x(I,J) + g + \sqrt{g^2 - 4h}} \right) \\ & = \lambda cf\Delta t \end{aligned}$$

$$[x(I,J)^2 + gx(I,J) + h]^\beta \cdot \left[\frac{2x(I,J) + g - \sqrt{g^2 - 4h}}{2x(I,J) + g + \sqrt{g^2 - 4h}} \right]^\gamma = e^{\lambda cf\Delta t} \quad (4.30b)$$

where

$$\begin{aligned} &= \frac{c}{2} \\ &= \left(1 - \frac{gc}{2}\right)(g^2 - 4h)^{-0.5} \end{aligned}$$

For a system for which the physical constant $D > 0$, Eqs. 4.19 through 4.21 can be solved by method of characteristics as per Chen et al. (1976).

Let

$$\bar{z} = z/v$$

and by the method of characteristics.

For characteristic I:

$$\frac{d\bar{z}}{dt} = 1$$

so that

$$\frac{dy}{d\bar{z}} = -\left(\frac{1-\epsilon}{\epsilon}\right)\lambda(y - y^*) \quad (4.19a)$$

For characteristic II:

$$\frac{d\bar{z}}{dt} = 0$$

and

$$\frac{dx}{dt} = \lambda(y - y^*) \quad (4.20a)$$

Applying the modified Euler method to Eqs. 4.19a and 4.20a, the following is obtained,

$$y(I, J) = y(I-1, J-1) - \left(\frac{1-\epsilon}{\epsilon}\right)\frac{\lambda}{2}\Delta t [y(I, J) - y^*(I, J) + y(I-1, J-1) - y^*(I-1, J-1)] \quad (4.19b)$$

and

$$x(I,J) = x(I,J-1) + \frac{\lambda}{2} \Delta t [y(I,J) - y^*(I,J) + y(I,J-1) - y^*(I,J-1)] \quad (4.20b)$$

where

$$\Delta t = \Delta \bar{z} = \frac{H}{Nz \cdot v}$$

and

$$y^*(I,J) = \frac{(A + D - B \cdot x(I,J))}{2B \cdot D} + \frac{\sqrt{[A + D - B \cdot x(I,J)]^2 + 4B \cdot D \cdot x(I,J)}}{2B \cdot D} \quad (4.23a)$$

For the system under consideration, Eqs. 4.19b, 4.20b and 4.23a along with the necessary external equations were used to calculate the concentration transients emerging from the column for the staged sequence cyclic process by iterative method.

Calculation of y^* --For the calculation of the fluid concentration in equilibrium with solid phase, y^* , the following constants were used:

	<u>O-Xylene</u>			<u>Anisole</u>		
	<u>303°K</u>	<u>333°K</u>	<u>358°K</u>	<u>303°K</u>	<u>333°K</u>	<u>358°K</u>
A:	8.65	1.46	8.00	1.40	9.00	8.25
B:	66.97	18.47	65.00	1.89	68.90	120.00

and

$$D = 0.29 \text{ cm}^3 \text{ pores/gm dry silica gel}$$

Calculation of λ_i . λ_i , the mass transfer coefficient, is a function of concentration and temperature, therefore values of λ_i must be calculated for every cell in the column. Kim (1976)

developed a set of equations for the calculation of mass transfer coefficients for the system toluene-acetophenone-n-heptane on silica gel. Stokes (1976) generalized the equations for multi-component systems. Stokes' equations were modified where necessary to suit the system O-xylene-anisole-n-heptane on silica gel.

$$\lambda_i = (A_p)(J_D)(v)(\epsilon)(Sc)^{-2/3} \quad (4.30d)$$

where

$$J_D = (Re)^{-0.78} \text{ for laminar flow}$$

$$Re = \frac{D_p v \rho_f \epsilon}{\mu_f (1 - \epsilon)} = \text{Reynolds No. for flow in packed beds}$$

$$Sc = \frac{\mu_f}{\rho_f D_f} = \text{Schmidt No.}$$

$$A_p = a_p / \rho_s = \text{interfacial area/unit weight of adsorbent}$$

$$v\epsilon = \text{superficial column velocity}$$

For staged sequence cyclic process, $v\epsilon$ can be expressed as follows:

	<u>Stage I</u>	<u>Stage II</u>	<u>Stage III</u>
Column 1	$(R+P_I+P_T)Qt_I$	$(R+P_I+P_B)Qt_{II}$	$(R+P_B)Qt_{III}$
Column 2	$(R+P_I+P_T)Qt_I$	$(R+P_I)Qt_{II}$	$(R+P_T+P_B)Qt_{III}$
Column 3	$(R+P_T)Qt_I$	$(R+P_I+P_B)Qt_{II}$	$(R+P_T+P_B)Qt_{III}$

where t_I , t_{II} , t_{III} = stage duration time for stage I, II and III respectively,

and

$$R = \text{reflux ratio}$$

$$\rho_f = \sum_{n=1}^n y_i M_i$$

$$\mu_f = \frac{\sum_{n=1}^n y_i \mu_i}{\sum_{n=1}^n y_i}$$

where

y_i = moles i /volume of solution

μ_i can be calculated from the Thomas' equation (Thomas, 1946).

$$\mu_i = 0.1167 \rho_\ell^{1/2} 10^\gamma$$

$$\gamma = \frac{B(1 - T_r)}{T_r}$$

μ_i = solute viscosity in centipoise

ρ_ℓ = solute density at normal boiling point, g/cc

B = viscosity constant to be calculated by summation of the atomic and group contributions

T_r = reduced temperature of solutes, expressed as a fraction of a given temperature to the critical temperature, $T^\circ\text{K}/T_c^\circ\text{K}$

	$T_c^\circ\text{K}$	B
n-Heptane	540	0.75
O-Xylene	625	0.7678
Anisole	642	0.8668

The following is the calculated viscosity data from Thomas' equation:

	<u>Viscosity in gm/cm.min)</u>		
	<u>303°K</u>	<u>333°K</u>	<u>358°K</u>
n-Heptane	0.2236	0.1694	0.1393
O-Xylene	0.4340	0.3125	0.2479
Anisole	0.6518	0.4453	0.3403

α which is functionally dependent on the solute and concentration (Kim, 1976), was shown to asymptotically approach a constant value at low concentration. The functional dependency of α on concentration was obtained via a curve fitting method for acetophenone and toluene and the equations are applicable to a good degree of accuracy to anisole and O-xylene.

The diffusivity, D_f , of the solute-solvent is a function of the solute and temperature as expressed by the modified equation of Wilke and Chang (1955) and can be estimated by

$$D_{fi} = \frac{7.4 \times 10^{-8} (60) (\psi_s M_s)^{0.5} T}{\mu_f V_{Mi}^{0.6}}$$

where

- D_{fi} = mutual diffusion coefficient of solute i at low concentrations in the solvent, cm^2/min
- ψ_s = association factor of solvent, dimensionless
= 1.0 for heptane (unassociated solvent)
- μ_f = viscosity of solvent, $\text{gm}/\text{cm}/\text{min}$
- M_s = solvent molecular weight, 100.2 gm/mole for heptane
- V_{Mi} = molal volume of solute i at normal boiling point $\text{cc}/\text{g mole}$

= 118.358 cc/g mole for O-xylene
 = 108.683 cc/g mole for anisole
 T = temperature of column, °K, $T_1(=30)$, $T_2(=60)$ or
 $T_3(=85)$

THE CELL (EFFECTIVE PLATE) MODEL (STOP & GO ALGORITHM)

The adsorbent bed is divided into N equal cells (plates or stages), each of length z/NNz , where z is the length of the column, and each stage is represented as i,j . In this case, i will be the cell number, and j is the transfer step. The schematic of this cell model is clearly depicted by Figure 4.1. Initially, the system is assumed to be in equilibrium at $j-1$, in which case each cell will have uniform concentrations in both the fluid and solid phases. If each fluid section is displaced exactly one step ahead in the transfer step, then the fluid $y(i,j-1)$ originally opposite the solid section i will now be opposite $i+1$. After each transfer step, the operation is stopped, and mass transfer is allowed to occur in all stages. Thereafter, equilibrium is immediately re-established and the next transfer step (j) begins.

COMPUTATION ALGORITHM

Continuous Parametric Pumping

The diagram of the operational steps used in the simulation of the parametric pumping process is depicted in Figure 4.2. Equations 4.16 was used in the calculation of all concentration transients. Divide the adsorbent columns into NZ equal stages,

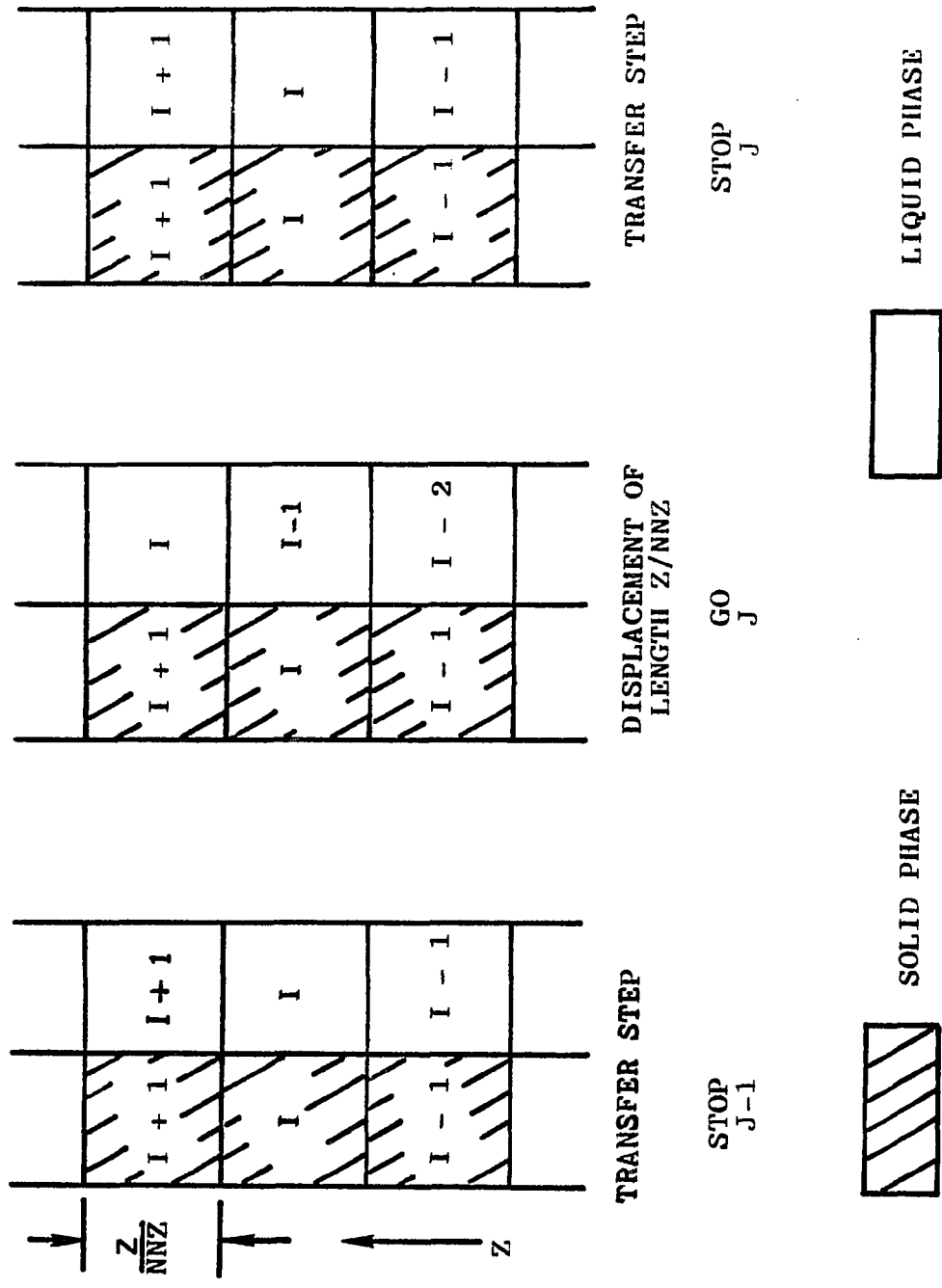


FIGURE 4.1 OPERATIONAL STEPS OF STOP & GO METHOD

each of length Z/NZ and Z being the length of the bed. Divide the time domain into NT increments. The time interval for the downward fluid flow is NT_1 , and NT_2 for the upward fluid flow.

Initialize the fluid and solid compositions in the NZ stages to some physically realizable values at $T_2(T_2 T_1)$. Initial composition was assumed to be $Y_{INT} = 1$ in this simulation. The initialization (equilibration) step is at $j = 1$ (see Figure 4.2(a)). The operational steps of the algorithm are as follows:

1. Push Down (Figure 4.2(b)): Columns 1 and 2 are operated at T_1 and T_2 respectively. The time step NT_1 for the downward flow of the fluid phase is divided into NZ equal time increments of length NT_1/NZ . Each fluid section is displaced one step ahead beginning at $j=2$ for each time element NT_1/NZ . A predetermined volume of feed is mixed with the fluid from the top reservoir and introduced into column 1, while top and bottom products are simultaneously withdrawn. Equilibration is allowed to re-establish, the concentration profile Y in the column is determined and another displacement is made; this time at $j=3$. When $j=NT_1$ time step is attained, the bottom reservoir concentration is calculated.
2. Push Up (Figure 4.2(c)): Columns 1 and 2 are now operated at T_2 and T_1 respectively. The time step NT_2 for the upward flow of the fluid phase is divided into NZ equal time increments of length NT_2/NZ . Each fluid section is displaced one step ahead beginning at $j=2$ for each time element

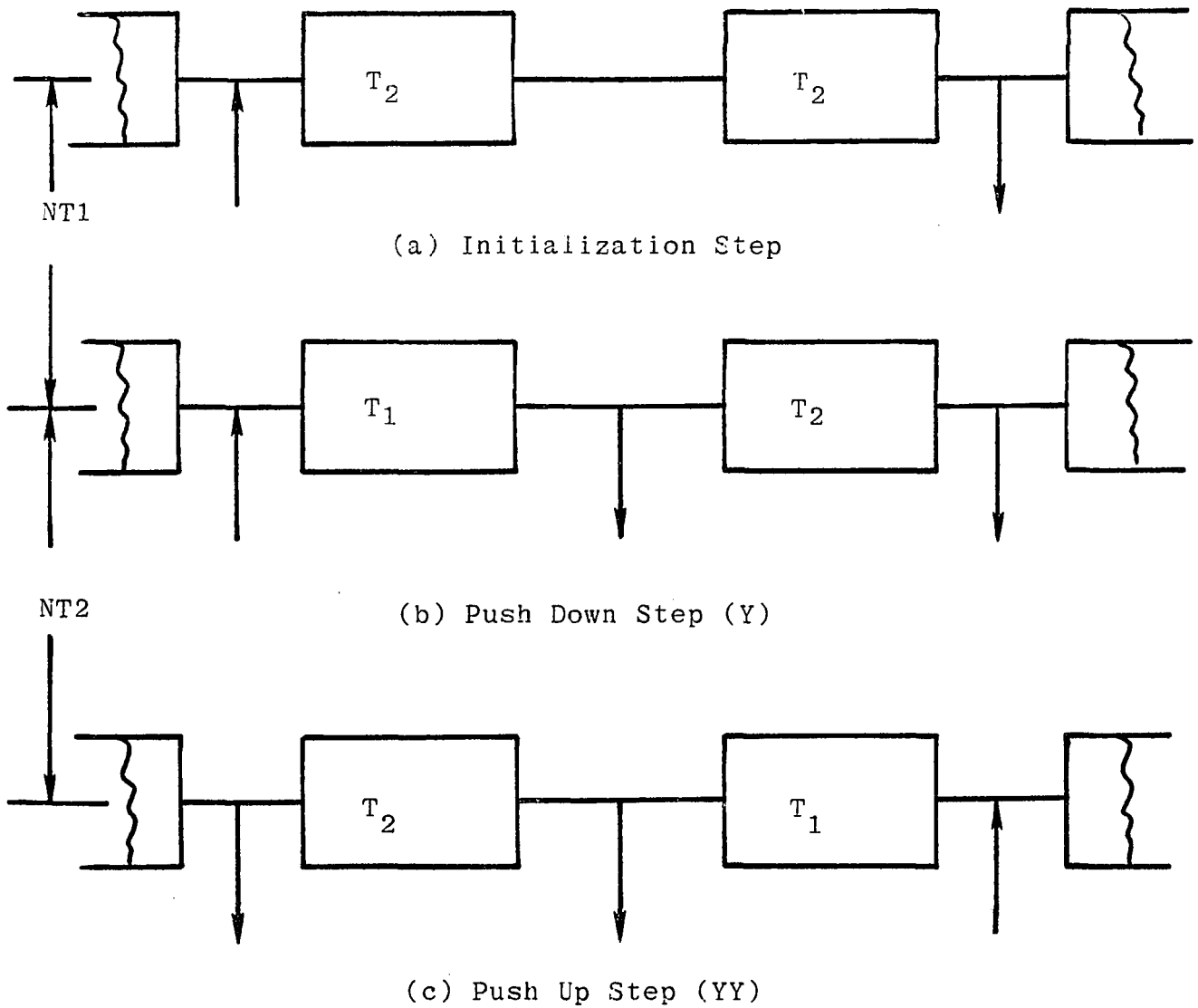


FIGURE 4.2 **DIAGRAM OF OPERATIONAL STEPS USED IN COMPUTER SIMULATION - CONTINUOUS PARAMETRIC PUMPING**

NT2/NZ. The mixture of feed and fluid from the bottom reservoir is now introduced into column 2 at T_1 , while top and bottom products are simultaneously withdrawn. Successive equilibration is allowed, and concentration profile YY determined until a final displacement at $j=NT2$ is attained, after which the top reservoir concentration is calculated.

This sequence of operation ends the first cycle. For subsequent cycles, steps 1 and 2 have to be repeated. The simulation of this calculational algorithm assumes the following:

- (a) That these NZ increments (volume elements) are entirely independent of one another.
- (b) That the calculation of concentration profiles of the fluid mixtures assume a set of pseudo-binary (all components are non-interactive, and non-reacting).
- (c) That the volume elements represent batch reactors connected in series.
- (d) That only partial equilibration between adjacent phases and full equilibration between opposite (solid and fluid) phases take place.
- (e) That each volume element is treated individually for calculating concentrations.

Appendix V contains a listing of the FORTRAN IV digital computer program written to implement the EQUILIBRIUM THEORY WITH STOP-GO METHOD for the direct mode parametric pumping.

CYCLIC ADSORPTION PROCESS

Stage I

1. Divide each adsorbent bed into NZ equal axial position increments and the stage duration time into NT time increments, such that $NZ/v = t$, $H(Nz*v)=t/NT$.
2. The system is initially assumed to be in equilibrium with the feed concentration at T_3 .
3. Calculate $y(I,J)$ and $x(I,J)$ by Eqs. 4.23a, 4.26a and 4.30c with the initial ($J=1$) and boundary ($I=1$) condition shown below:

Initial Conditions:

For each column, $y(I,1)_n = y(I,NT)_{n-1/3}$ = concentration of y at the end of $(n-1/3)$ th stage, n = number of complete cycle.

$x(I,1)_n = x(I,NT)_{n-1/3}$ = concentration of x at the end of $(n-1/3)$ th stage.

$$\lambda(I,1) = f[y(I,1)_n] \text{ via Eq. 4.30d}$$

and

$$y^*(I,1) = f[x(I,1)_n] \text{ via Eq. 4.23a}$$

Boundary Conditions:

$$x(1,J)|_{n-1/3} = x(1,J-1)|_{n-1/3} + \Delta x$$

where Δx is the increment in x obtainable by the fourth order Runge-Kutta numerical integration of Eq. 4.20,

$$K_1 = \lambda(y_0 - y_0^*)\Delta t$$

let

$$x_1 = x_0 + K_1/2$$

$$K_2 = \lambda(y_0 - y_1^*)\Delta t$$

$$y_1^* = f(x_1) \text{ via Eq. 4.21}$$

$$x_2 = x_0 + K_2/2$$

$$K_3 = \lambda(y_0 - y_2^*)\Delta t, \quad y_2^* = f(x_2)$$

$$x_3 = x_0 + K_3$$

$$K_4 = \lambda(y_0 - y_3^*)\Delta t, \quad y_3^* = f(x_3)$$

therefore

$$\Delta x = 1/6(K_1 + 2K_2 + 2K_3 + K_4)$$

4. Calculate $y(I,J)$ and $x(I,J)$ for $t = \Delta t, 2\Delta t, 3\Delta t, \dots, NT\Delta t$, and $\bar{z} > 0$, by performing the following steps:

Step 1: Estimate values for $y(I,J)$ and $x(I,J)$ as follows:

$$y(I,J)^{es} = y(I-1,J-1)$$

$$-\left(\frac{1-\epsilon}{\epsilon}\right)\lambda(I-1,J-1)[y(I-1,J-1)-y^*(I-1,J-1)] \cdot NT \cdot \Delta t$$

and

$$x(I,J)^{es} = x(I,J-1) + \lambda(I,J-1)[y(I,J-1)-y^*(I,J-1)] \cdot NT \cdot \Delta t$$

Step 2: Using estimated values of $y(I,J)$ and $x(I,J)$ to calculate $y^*(I,J)^{es}$ and $\lambda(I,J)^{es}$ from Eqs. 4.23a and 4.30d respectively.

Step 3: We are now in a position to calculate the concentrations from Eqs. 4.19b and 4.20 b by using estimated values,

$$\begin{aligned}
 y(I,J) &= y(I-1,J-1) \\
 &\quad - \left(\frac{1-\epsilon}{\epsilon}\right) \frac{\Delta t}{2} \lambda(I,J) \epsilon s [y(I,J) \epsilon s - y^*(I,J) \epsilon s] \\
 &\quad - \left(\frac{1-\epsilon}{\epsilon}\right) \frac{\Delta t}{2} \lambda(I-1,J-1) [y(I-1,J-1) - y^*(I-1,J-1)]
 \end{aligned}$$

and

$$\begin{aligned}
 x(I,J) &= x(I,J-1) \\
 &\quad + \frac{\Delta t}{2} \lambda(I,J) \epsilon s [y(I,J) \epsilon s - y^*(I,J) \epsilon s] \\
 &\quad + \frac{\Delta t}{2} \lambda(I,J-1) [y(I,J-1) - y^*(I,J-1)]
 \end{aligned}$$

Step 4: Check for deviation between values from steps 1 and 3,

$$\left| \frac{y(I,J) - y(I,J) \epsilon s}{y(I,J) \epsilon s} \right| \leq \epsilon$$

and

$$\left| \frac{x(I,J) - x(I,J) \epsilon s}{x(I,J) \epsilon s} \right| < \epsilon$$

where ϵ is the desired tolerance.

If the conditions specified in this step are not satisfied, repeat steps 1 through 4.

For subsequent stages, repeat the procedure from number 3 to 4 (see Figure 4.3).

Appendix V contains a listing of the FORTRAN IV digital computer program written to implement the calculational algorithm for the staged sequence cyclic adsorption process.

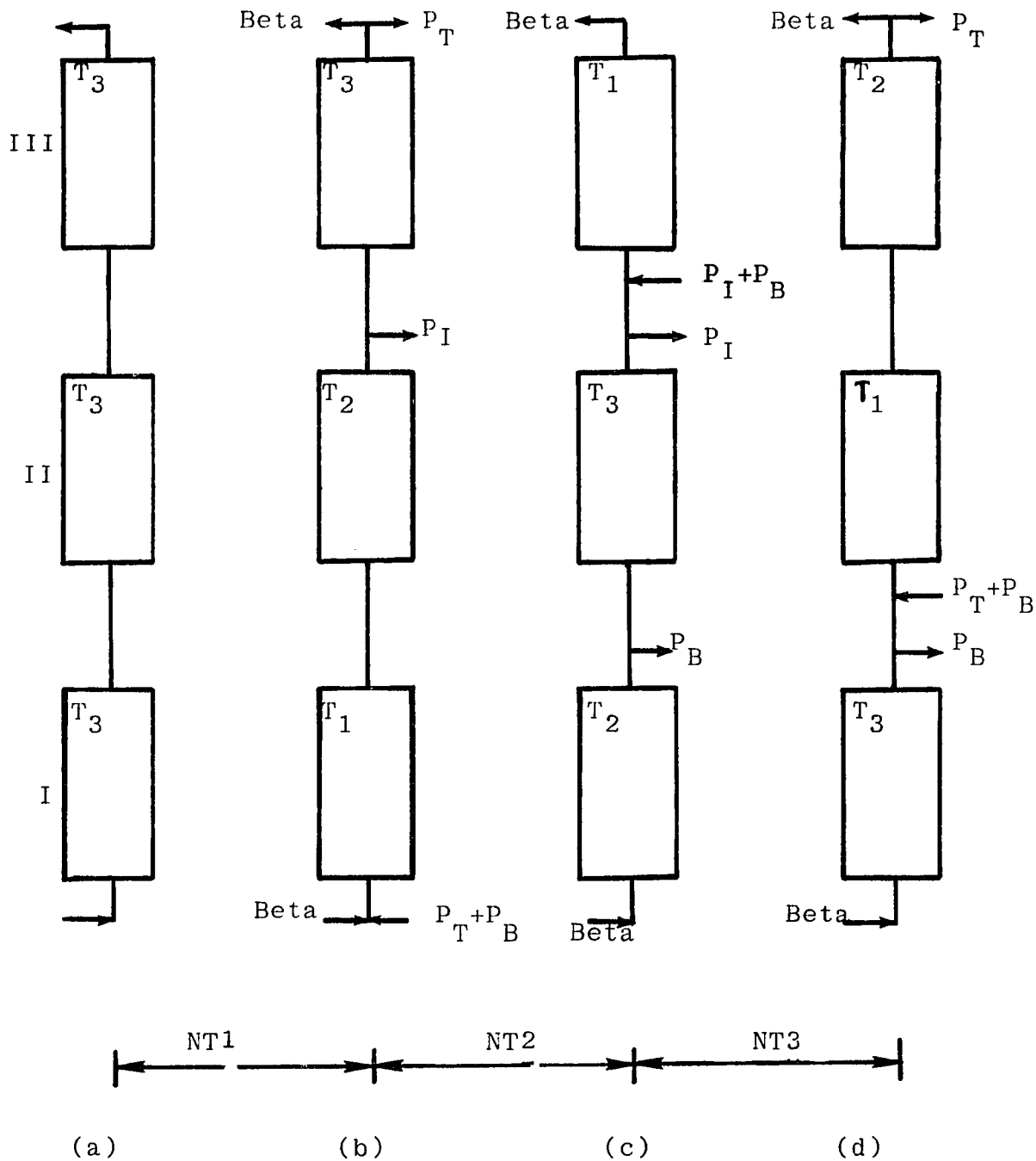


FIGURE 4.3 SCHEMATIC DESCRIPTION OF THE OPERATIONAL STEPS USED IN THE COMPUTER SIMULATION OF THE STAGED SEQUENCE CYCLIC ADSORPTION PROCESS.
 (a) INITIALIZATION STEP (b) STAGE I (c) STAGE II
 (d) STAGE III

SOLUTION BY METHOD OF CHARACTERISTICS

Material Balance with Finite Mass-Transfer Rate

Let us go back to the material balance equations (Eqs. 4.19 and 4.20), but we will now assume that y^* in the finite mass-transfer rate between mobile and stationary phases expressed by the flux $\lambda(y-y^*)$ is linear (see Eq. 4.31) instead of the non-linear Langmuir isotherm expressed by Eq. 4.21. For clarity the basic equations will be presented again.

$$\frac{\partial y}{\partial t} + \frac{v}{\epsilon} \frac{\partial y}{\partial z} = - \lambda(y - y^*) \quad (4.19)$$

$$\frac{\partial x}{\partial t} = \left(\frac{\epsilon}{1 - \epsilon} \right) \lambda(y - y^*) \quad (4.20)$$

$$y^* = x/k(T) \quad (4.31)$$

Chen et al. (1976) and Stokes (1976) each independently presented a numerical scheme for solving the material balance equations by the method of characteristics. We will again assume that all physical properties are constant. The fluid entering the column is also assumed to be at constant compositions and velocity. The solutions to Eqs. 4.19 and 4.20 can be expressed in the form of

$$y(u_1, u_2) = 0 \text{ and } x(u_3) = 0 \quad (4.32)$$

where

$$u_1(t, z) = c_1, u_2(t, z) = c_2 \text{ and } u_3(t) = c_3 \quad (4.33)$$

The natural boundary conditions to specify are

$$x(z, 0) = x_0 \quad 0 \leq z \leq L \quad (4.34)$$

$$y(z, 0) = y_0 \quad 0 \leq z \leq L \quad (4.35)$$

$$y(0, t) = \langle y \rangle \quad t \geq 0 \quad (4.36)$$

$$\frac{dx(0, t)}{dt} = \lambda(\langle y \rangle - y^*), \quad t \geq 0 \quad (4.36a)$$

Equation 4.36 implies that at the entrance of the column, $\langle y \rangle$ represents an average concentration which could constitute combination of the feed solution ($y_0=1$) and the reflux solutions.

According to the method of characteristics (Acrivos, 1956), the choice of paths in the (z, t) -plane is optional. Equations 4.32 and 4.33 are independent solutions of two of the associated ordinary equations

$$\frac{dt}{1} = \frac{dz}{v/\epsilon} = - \frac{dy}{\lambda(y - x/k)} \quad (4.37)$$

and

$$\frac{dt}{1} = \frac{dz}{0} = \frac{1 - \epsilon}{\epsilon} \frac{dx}{\lambda(y - x/k)} \quad (4.38)$$

Since the characteristic curves are straight lines with direction ratios (t, z, y) and (t, x) , it then follows that any surface (Eqs. 4.32 and 4.33) contains the straight lines from the origin to points on the surface. Although the geometric interpretation of the solutions of Eqs. 4.19 and 4.20 can readily be obtained, an explicit solution of a pair of the associated equations (Eq. 4.37 or 4.38) could be difficult.

Equality of the first two members of Eq. 4.37 gives

$$\frac{dz}{dt} = \frac{v}{\epsilon} \quad (4.39)$$

and equality of the last two members of Eq. 4.37 gives

$$\frac{dy}{dz} = - \frac{\lambda \epsilon (\bar{y} - x/k)}{v} \quad (4.40)$$

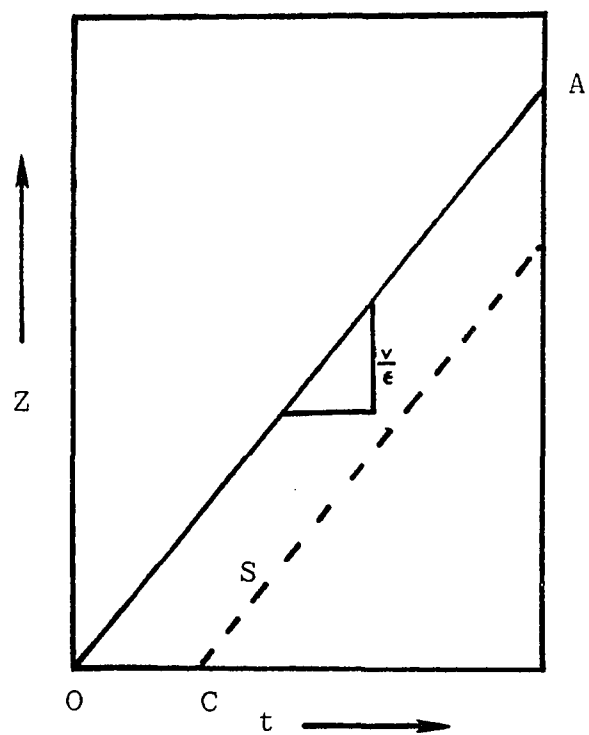


FIGURE 4.4 Z, t -PLANE ALONG WHICH $Y(Z, t)$ IS DEFINED

As shown in Fig. 4.4, the characteristics are straight lines in the (z,t) -plane of slope v/ϵ (Eq. 4.39). Consider a point (z,t) lying on or parallel to OA, that is

$$(t - c) > \frac{\epsilon z}{v} .$$

where c is the distance of any family of curves parallel to the OA. The inclination of the characteristics is

$$\theta = \tan^{-1} \left(\frac{v}{\epsilon} \right)$$

If $c = t - \epsilon z/v$, then to find S the following derivations are necessary.

$$ds^2 = dz^2 + dt^2$$

$$ds^2 = dz^2 \left(1 + \left[\frac{dt}{dz} \right]^2 \right)$$

Therefore,

$$s = \frac{z}{v} \sqrt{v^2 + \epsilon^2} \quad (4.41)$$

Rewriting Eq. 4.40 in terms of the arbitrary variable s ,

$$\frac{dy}{ds} \cdot \frac{ds}{dz} = - \frac{\lambda \epsilon (y - x/k)}{v}$$

but

$$\frac{ds}{dz} = \frac{\sqrt{v^2 + \epsilon^2}}{v}$$

Therefore

$$\frac{dy}{ds} = - \frac{\lambda \epsilon (y - x/k)}{\sqrt{v^2 + \epsilon^2}}$$

or

$$\frac{dy}{ds} + \frac{\lambda \epsilon}{\sqrt{v^2 + \epsilon^2}} y = \frac{\lambda \epsilon}{\sqrt{v^2 + \epsilon^2}} \frac{x}{k} \quad (4.42)$$

and the solution to Eq. 4.42 is the sum of the complimentary and particular solutions.

$$y(c,s) = A_1 \exp\left(-\frac{\lambda \epsilon s}{\sqrt{v^2 + \epsilon^2}}\right) + \frac{x}{k}$$

or

$$y(z,t) = A_1 \exp\left(-\frac{\lambda \epsilon}{v} z\right) + \frac{x}{k} \quad (4.43)$$

Application of the boundary condition of Eq. 4.22 yields

$$y(z,t) = \frac{x}{k} + (\langle y \rangle - x/k) \exp\left(-\frac{\lambda \epsilon z}{v}\right) \quad (4.44)$$

In the same fashion, equality of the first two members of Eq. 4.38 gives

$$\frac{dz}{dt} = 0 \quad (4.45)$$

and equality of the last two members of Eq. 4.38 yields

$$\frac{dx}{dt} = \frac{\epsilon \lambda (y - x/k)}{(1 - \epsilon)} \quad (4.46)$$

As depicted by Fig. 4.5, the characteristics of the solid phase concentration, x , are straight lines in the (z,t) -plane with slope 0 or $z = \text{constant}$. Upon integration of Eq. 4.46, we obtain

$$t = -\frac{k(1 - \epsilon)}{\epsilon \lambda} \ln (y - x/k) + A_2 \quad (4.47)$$

Applying the boundary condition of Eq. 4.34 and 4.35, the following expression is obtained

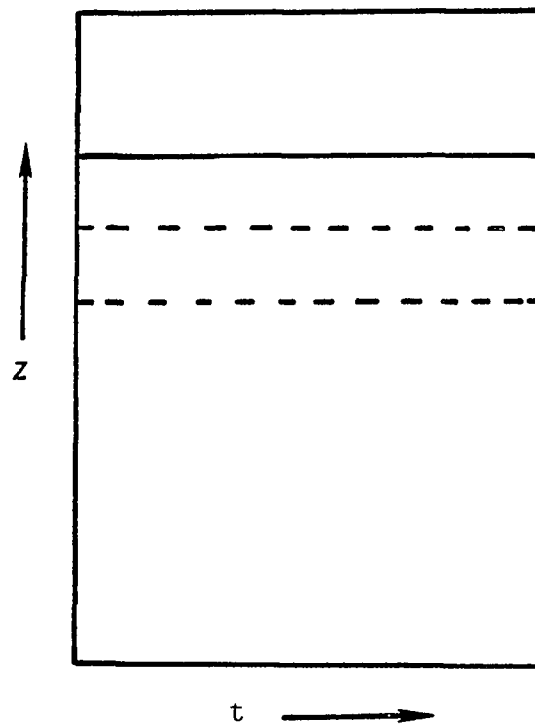


FIGURE 4.5 z, t -PLANE ALONG WHICH $X(z, t)$ IS DEFINED

$$x(z, t) = k \left[y - B e^{-\left(\frac{\epsilon}{1-\epsilon}\right) \frac{\lambda t}{k}} \right] \quad (4.48)$$

where $B = y_0 - x_0/k$

To calculate $x(z, t)$ and $y(z, t)$ at the points where the two characteristics intersect, we substitute Eq. 4.48 into Eq. 4.44 to obtain

$$y = \frac{1}{B} \left[B y - e^{-\left(\frac{1-\epsilon}{\epsilon k}\right) \lambda t} \right] \left[1 - e^{-\frac{\lambda \epsilon z}{v}} \right] + \langle y \rangle e^{-\frac{\lambda \epsilon z}{v}}$$

and upon simplification, we get

$$y(z, t) = \langle y \rangle + B \left\{ e^{-\frac{\epsilon \lambda t}{(1-\epsilon)k}} - e^{-\left[\frac{\epsilon \lambda t}{(1-\epsilon)k} - \frac{\lambda \epsilon z}{v}\right]} \right\} \quad (4.49)$$

If we now substitute Eq. 4.49 into Eq. 4.48, an expression can be obtained for $x(z, t)$.

$$x(z, t) = k \left\{ \langle y \rangle - B e^{-\left[\frac{\epsilon \lambda t}{(1-\epsilon)k} - \frac{\lambda \epsilon z}{v}\right]} \right\} \quad (4.50)$$

Note that Eqs. 4.49 and 4.50 are only defined at the points where the characteristics intersect.

From Eqs. 4.48 and 4.49 the fluid phase concentration $y(z, t)$ can be obtained along with the characteristic $z = vt/\epsilon + c$ and the solid phase concentration $x(z, t)$ can also be obtained along the characteristic $z = c$. The values of $y(z, t)$ and $x(z, t)$ during the parapumping process are functionally dependent on many adjustable parameters: λ , k , t , z and v . From Eq. 4.49 it is apparent that for large bulk fluid velocity v , $y(z, t) \approx \langle y \rangle$, meaning that the concentration in the fluid phase before exiting the column will be essentially equal to the concentration of fluid that was pumped into the column. This phenomena is physically sound since mass-transfer from the fluid phase to the solid phase is significantly reduced for high velocities. As cycle time increases, $y(z, t)$ decreases and $x(z, t)$ increases for low temperature and vice versa for high temperatures which is what should be ex-

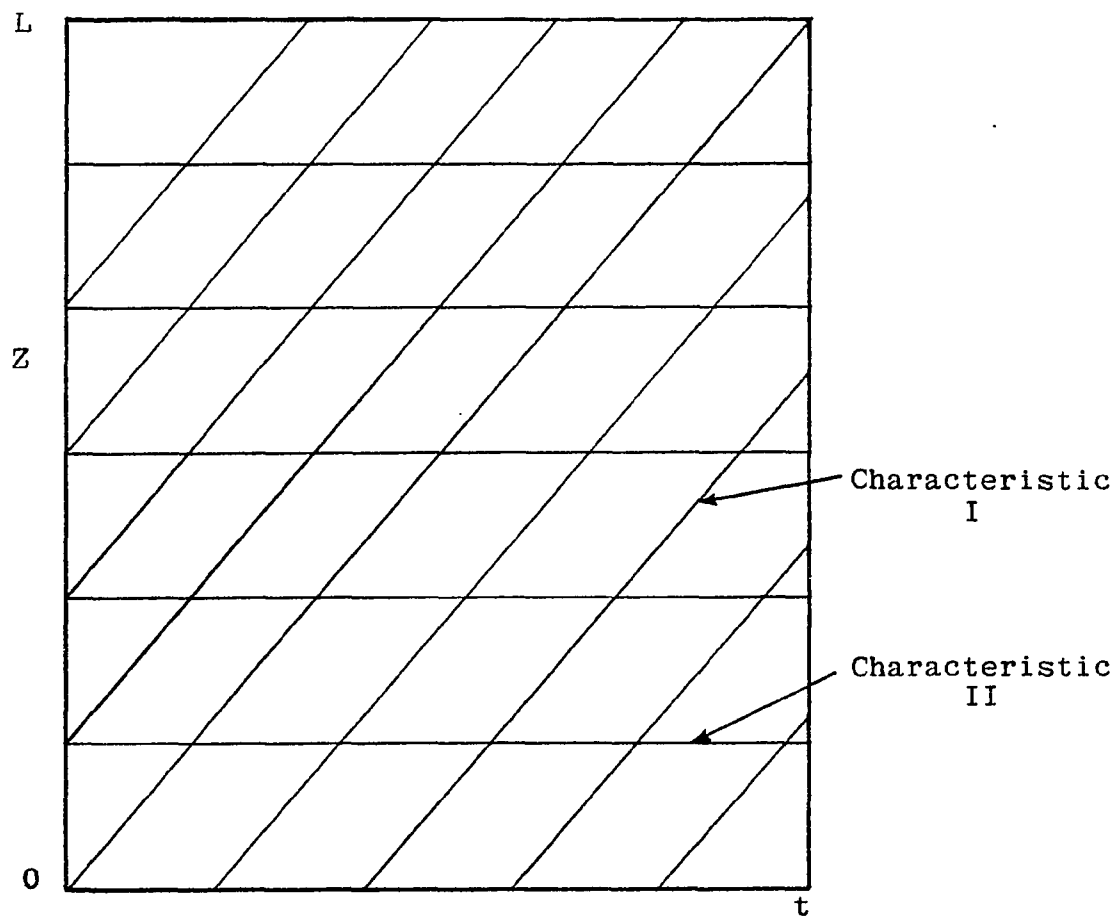


FIG. 4.6 : STEADY STATE CHARACTERISTICS FOR BATCH PARAMETRIC PUMPING

CHARACTERISTICS I: FLUID PHASE

CHARACTERISTICS II: SOLID PHASE

pected, since longer times allow for near equilibrium situations to be attained and mass-transfer from the fluid phase into the solid phase to occur for low temperatures (mass-transfer from the solid phase into the fluid phase is obtained for high temperatures).

Equations 4.49 and 4.50 can further be written to be independent of z and v , if $t = z/v$, we have

$$y(z, t) = \langle y \rangle + B \{ e^{-pqt} - e^{-[1-q]pt} \} \quad (4.51)$$

and

$$x(z, t) = k \{ \langle y \rangle - B e^{-[1-q]pt} \} \quad (4.52)$$

where

$$p = \lambda \epsilon \quad \text{and} \quad q = \frac{1}{(1 - \epsilon)k}$$

The parameter p characterizes the capacity of the fluid phase while the parameter q characterizes the capacity of the solid phase.

Instantaneous Mass-Transfer (Equilibrium Theory)

In Chapter 5, various criteria necessary to achieve the desired separations are developed by the method of characteristics based on the assumption of instantaneous mass-transfer between the fluid phase and the solid phase. Pigford et al. (1969), in the development of the equilibrium theory for processes inside the column assumed that local interphase equilibrium exists with a linear distribution law having a temperature-dependent distribution coefficient. Other pertinent as-

assumptions are negligible axial diffusion, instantaneous temperature change when the column temperature is changed, the existence of plug flow and constant fluid density. Chen et al. (1974) analyzed the separation of multicomponent mixtures by treating the mixtures as n pairs of pseudo-binary systems. Each system was assumed to include one solute and a common inert solvent. They characterized the system by an equilibrium parameter b_i , associated with a given two-phase system operated at two specific temperatures. The equilibrium parameter was expressed as

$$b_i = \frac{0.5(m_{2i} - m_{1i})}{1 + 0.5(m_{1i} + m_{2i})} \quad (4.53)$$

where

m_{1i} = dimensionless equilibrium constant at temperature T_1 for component i ;

m_{2i} = dimensionless equilibrium constant at T_2 for component i .

For three temperatures, b_i needs to be redefined as

$$b^1_i = \frac{m_{2i} - m_{1i}}{2 + m_{1i} + m_{2i}} \quad (4.54)$$

$$b^2_i = \frac{m_{3i} - m_{2i}}{2 + m_{2i} + m_{3i}} \quad (4.55)$$

where b^1_i is the equilibrium parameter associated with T_1 and T_2 , and b^2_i is the equilibrium parameter associated with T_2 and T_3 ($T_1 < T_2 < T_3$). Equation 4.53 is applicable to parametric pumping process where the pump is operated at two specific temperatures and Eqs. 4.54 and 4.55 are applicable to cyclic adsorption

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where

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m_{2i} = dimensionless equilibrium constant at T_2 for component i .

For three temperatures, b_i needs to be redefined as

$$b^1_i = \frac{m_{2i} - m_{1i}}{2 + m_{1i} + m_{2i}} \quad (4.54)$$

$$b^2_i = \frac{m_{3i} - m_{2i}}{2 + m_{2i} + m_{3i}} \quad (4.55)$$

where b^1_i is the equilibrium parameter associated with T_1 and T_2 , and b^2_i is the equilibrium parameter associated with T_2 and T_3 ($T_1 < T_2 < T_3$). Equation 4.53 is applicable to parametric pumping process where the pump is operated at two specific temperatures and Eqs. 4.54 and 4.55 are applicable to cyclic adsorption

process where more than two temperatures are needed for the fractionation of fluid mixtures. In general, for a sequential temperature input the equilibrium parameter associated with temperatures T_j and T_{j+1} may be expressed as

$$b_i^j = \frac{m_i(T_{j+1}) - m_i(T_j)}{2 + m_i(T_j) + m_i(T_{j+1})} \quad (4.56)$$

where

$$i = 1, 2, 3, \dots$$

$$j = 1, 2, 3, \dots$$

The material balance equations for the equilibrium theory will not be derived here (see Eqs. 5.1 through 5.8). The steady state characteristic solutions for parametric pumping and cyclic adsorption process will be tested separately. Let us consider the parametric pumping process for the separation of multicomponent mixtures (see Fig. 4.7)

PARAMETRIC PUMPING

$$u_{icon} = \frac{v}{1 + m_i(T)} \quad (4.57)$$

where

v = the bulk velocity of the mobile phase

u_{icon} = the velocity of the concentration wave of component i .

The slopes of the characteristics can then be written in terms of the interstitial velocity and the equilibrium parameter b_i ,

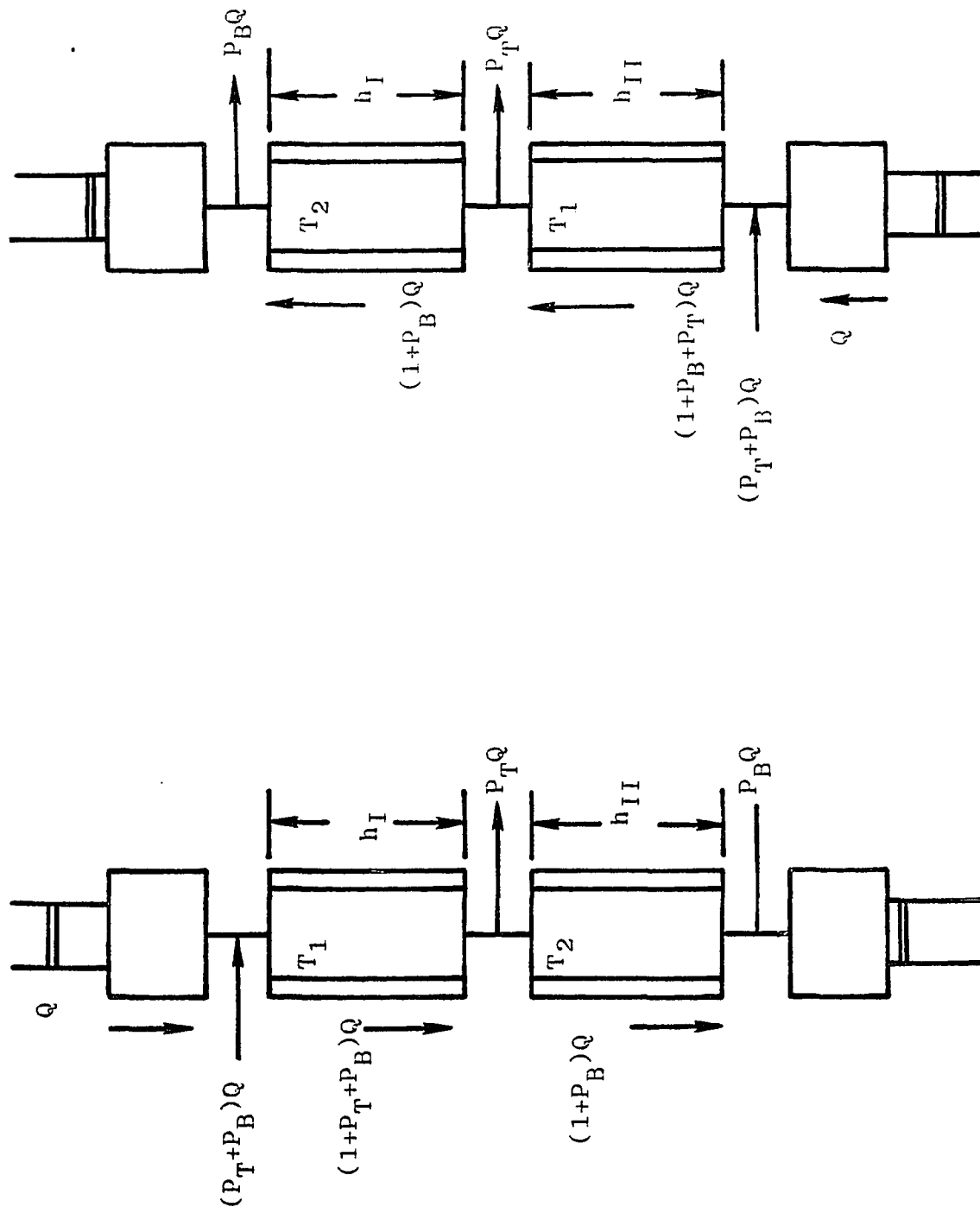


FIGURE 4.7 ALTERNATING TOP AND BOTTOM FEED ARRANGEMENT FOR A CONTINUOUS PARAMETRIC PUMP

Column I

$$\begin{aligned} \text{Downwards Cold Half Cycle} = u_{i, \text{con}} &\equiv \left(\frac{\partial z}{\partial t}\right)_c = \\ &= \frac{v_o(1 + P_T + P_B)}{(1 + b_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \end{aligned} \quad (4.58)$$

$$\begin{aligned} \text{Upwards Hot Half Cycle} = u_{i, \text{con}} &\equiv \left(\frac{\partial z}{\partial t}\right)_H = \\ &= \frac{v_o(1 + P_B)}{(1 - b_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \end{aligned} \quad (4.59)$$

Column II

$$\begin{aligned} \text{Downwards Hot Half Cycle} = u_{i, \text{con}} &\equiv \left(\frac{\partial z}{\partial t}\right)_H = \\ &= \frac{v_o(1 + P_B)}{(1 - b_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \end{aligned} \quad (4.60)$$

$$\begin{aligned} \text{Upwards Cold Half Cycle} = u_{i, \text{con}} &\equiv \left(\frac{\partial z}{\partial t}\right)_c = \\ &= \frac{v_o(1 + P_T + P_B)}{(1 + b_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \end{aligned} \quad (4.61)$$

Equations 4.57 through 4.61 are the concentration velocities for component i . The derivations are based on material balances in a volume element of the column. According to Eqs. 4.58 through 4.61, the mobile phase concentration velocity depends on the operating conditions and the equilibrium parameters $m_i(T)$ and $b_i(T)$, where, in terms of the nomenclature used by Pigford et al. (1969) and Chen et al. (1973),

$$m(T_2) = m_o - a$$

$$m(T_1) = m_o + a \quad (4.62)$$

$$b = a/(1 + m)$$

Equation 4.62 is the dimensionless equilibrium constant parameter for a single component, and to extend Eq. 4.62 to multi-component mixtures, Chen et al defined b_i as given by Eq. 4.53 for two specific temperatures where the constants a and m_{i0} (Eq. 4.62) now become,

$$a = \frac{m_i(T_2) - m_i(T_1)}{2} \quad (4.63)$$

$$m_{i0} = \frac{m_i(T_1) + m_i(T_2)}{2}$$

The characteristic lines are described by the distance-time derivatives (Eqs. 4.58 to 4.61), or

$$\frac{dz}{dt} = \frac{v}{1 + m(T)} = u_{i,con} \quad (4.64)$$

and

$$y(1 + m(T)) = \text{constant} \quad (4.65)$$

From Fig. 4.7 we know that

Downflow

$$h_I: (1 + P_T + P_B)Q = (1 + P_T + P_B)v_0A \quad (4.66)$$

$$h_{II}: (1 + P_B)Q = (1 + P_B)v_0A \quad (4.67)$$

Upflow

$$h_I: (1 + P_B)Q = (1 + P_B)v_0A \quad (4.68)$$

$$h_{II}: (1 + P_T + P_B)Q = (1 + P_T + P_B)v_0A \quad (4.69)$$

where

A = cross sectional area of the column

If Eqs. 4.66 to 4.69 and Eq. 4.53 are substituted into Eq. 4.64, Eqs. 4.58 through 4.61 are obtained. Eqs. 4.64 and 4.65 are obtained from the material balance equations as will be fully explained in Chapter 5. Equation 4.65 implies that the concentration along a characteristic line given by the slope $v/(1+m(T))$ (Eq. 4.64) are constant for any given temperature except at the boundary where the temperature is switched from one temperature to another. Therefore a change in concentration will accompany a change in temperature according to the following

$$\frac{y(T_1)}{y(T_2)} = \frac{1 - b_i}{1 + b_i} \quad (4.70)$$

A set of equations describing the characteristic lines in one column is adequate, provided the heights of both columns are equal (i.e. $h_I = h_{II}$), to fully describe the system (see Fig. 4.7) since the two columns are operated back to back. Now, if Eqs. 4.58 and 4.59 are integrated between the limits of $t=t_1$ and $t=t_2$ we get the wave front penetration distances for cold downflow and hot upflow (Column I), respectively, a concept first defined by Chen and Hill (1971).

$$L_i(T_1) = \frac{v_o(1 + P_T + P_B)\Delta t}{(1 + b_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \quad (4.71)$$

and

$$L_i(T_2) = - \frac{v_o(1 + P_B)\Delta t}{(1 - b_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \quad (4.72)$$

$$\frac{L_i(T_2)}{L_i(T_1)} = \frac{(1 + P_B)(1 + b_i)}{(1 + P_T + P_B)(1 - b_i)} \quad (4.73)$$

In the derivation of the concentration transients, Chen and Hill (1971a) presented the concentration transients for the top and bottom product streams for operation in Regions 1, 2 and 3. The equations predicted that, at steady state ($n \rightarrow \infty$), solute removal from the lower stream is complete in Region 1, but only partially removed in Regions 2 and 3. For the derivation of the concentration transients for the parapumping arrangements shown in Fig. 4.7, Region 1 mode of operation is applicable. The derivation of the concentration transients for the pseudo-binary system is based on the assumption that the less adsorbed solute acts as an inert solvent. This assumption is sound physically if the low temperature is chosen such that adsorption on the solid phase is minimal. Hence, the ternary system can then be treated as a pseudo-binary system.

If the feed is introduced into the top of the column during downflow, and $L_i(T_2) \geq L_i(T_1)$, then from Eq. 4.73 we have

$$\frac{L_i(T_2)}{L_i(T_1)} \geq \left(\frac{1 + P_B}{1 + P_T + P_B} \right) \left(\frac{1 + b_i}{1 - b_i} \right)$$

If we let

$$\left(\frac{1 + P_B}{1 + P_T + P_B} \right) \left(\frac{1 + b_i}{1 - b_i} \right) \geq 1 \quad (4.74)$$

This means that

$$\frac{1 + P_B}{P_T} \geq \frac{(1 - b_i)}{2b_i}$$

or

$$\frac{P_T}{1 + P_B} < \frac{2b_i}{1 - b_i} \quad (4.75)$$

if

$$\frac{P_T}{1 + P_B} = \frac{2b_i}{1 - b_i}$$

then

$$\frac{1 + P_B + P_T}{1 + P_B} = \frac{1 - b_i + 2b_i}{1 - b_i} = \frac{1 + b_i}{1 - b_i} \quad (4.76)$$

Equation 4.75 means that for the strongly adsorbed solute to concentrate at the top of the column (i.e. $L_i(T_2) > L_i(T_1)$), the ratio $P_T/(1+P_B)$ must be less or equal to $2b_i/(1-b_i)$. Another useful identity is given by Eq. 4.76.

Figure 4.8 shows top products exit during the n cycle of operation. The external equation may be obtained from material balance based on Fig. 4.8. By making a solute and total mass balance, the following relation for the n^{th} downflow half-cycle may be obtained:

$$\langle y_{T2} \rangle_n (1 + P_T + P_B) = \langle y_T \rangle_{n-1} (1 + P_B) \quad (4.77)$$

Upon substituting Eq. 4.76 into Eq. 4.77 and rearranging the resulting equation, the following is obtained:

$$\langle y_{T2} \rangle_n = \frac{1 - b_i}{1 + b_i} \langle y_{T1} \rangle_{n-1} \quad (4.78)$$

During the $(n-1)$ th cycle (i.e. upflow half cycle), the fluid emerging from the bottom column experiences a change in concentration equal to

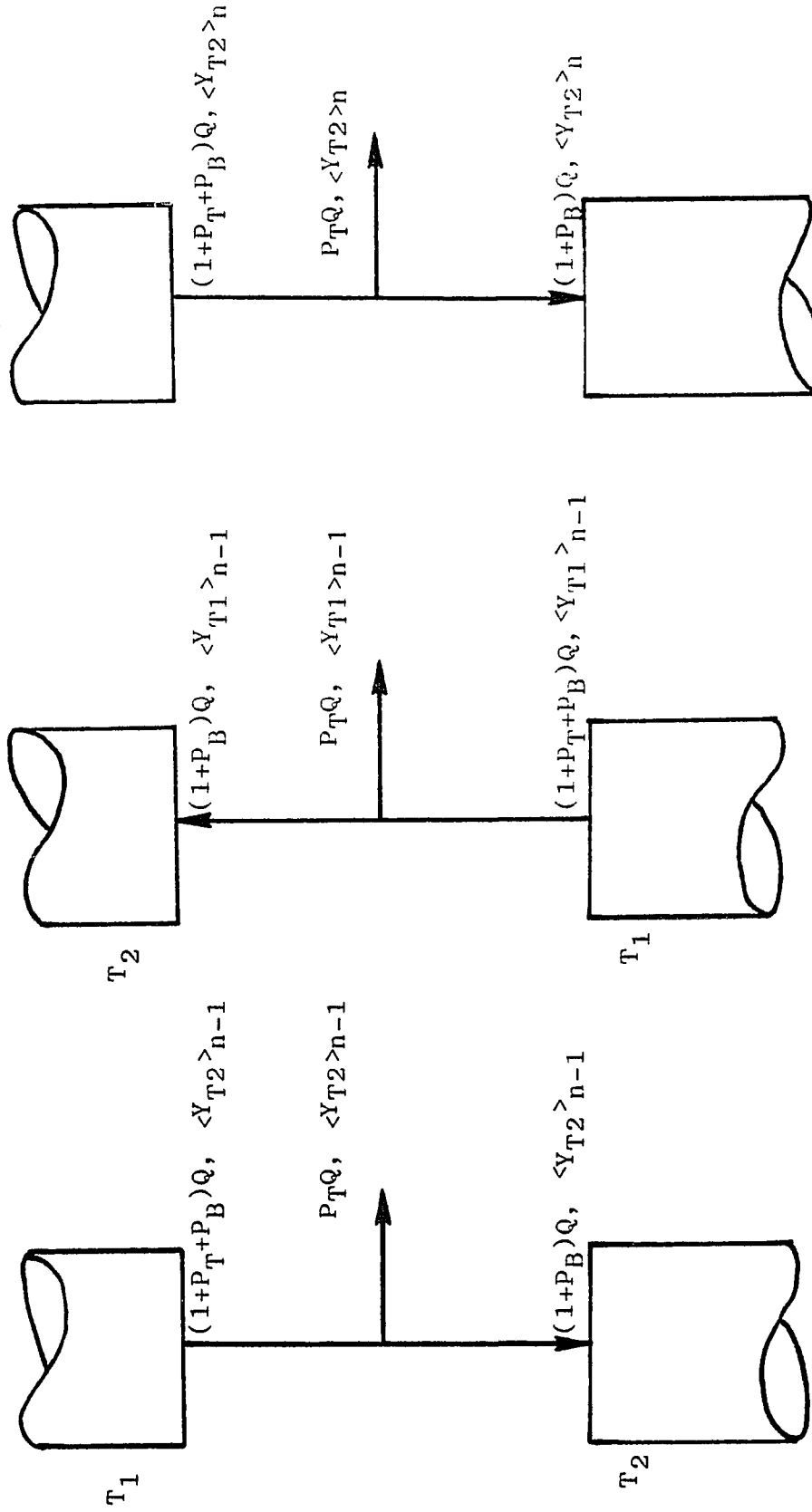


FIGURE 4.8 EXTERNALS FOR MIDDLE SECTION OF TWO COLUMN PARAMETRIC PUMP WITH ALTERNATING TOP AND BOTTOM FEED

$$\langle y_{T1} \rangle_{n-1} = \left(\frac{1 - b_i}{1 + b_i} \right) \langle y_{T2} \rangle_{n-1} \quad (4.79)$$

and Eq. 4.78 now becomes

$$\langle y_{T2} \rangle_n = \left\{ \left(\frac{1 - b_i}{1 + b_i} \right) \left(\frac{1 - b_i}{1 + b_i} \right) \right\} \langle y_{T2} \rangle_{n-1}, \quad n \geq 2 \quad (4.80)$$

or

$$\langle y_{T2} \rangle_n = \left\{ \left(\frac{1 - b_i}{1 + b_i} \right)^2 \right\}^{n-1} \langle y_{T2} \rangle_1$$

I.C. at $n = 1$,

$$\langle y_{T2} \rangle_1 = y_0$$

Therefore

$$\langle y_{T2} \rangle_n = y_0 \left(\frac{1 - b_i}{1 + b_i} \right)^{2n-2}$$

or

$$\frac{\langle y_{T2} \rangle_n}{y_0} = \left(\frac{1 - b_i}{1 + b_i} \right)^{2n-2} \quad (4.81)$$

By means of Eq. 4.81, the concentration transients can be calculated during the downflow half cycle, and for the upflow half cycle, the following equation can be used in calculating the concentration transients,

$$\frac{\langle y_{T1} \rangle_n}{y_0} = \left(\frac{1 - b_i}{1 + b_i} \right) \left(\frac{1 - b_i}{1 + b_i} \right)^{2n-2} = \left(\frac{1 - b_i}{1 + b_i} \right)^{2n-1} \quad (4.82)$$

Since $b_i \ll 1$, at steady state ($n \rightarrow \infty$), Eqs. 4.81 and 4.82 become

$$\frac{\langle y_{T2} \rangle_\infty}{y_0} \text{ or } \frac{\langle y_{T1} \rangle_\infty}{y_0} = 0 \quad (4.83)$$

Equation 4.83 means that at steady state, the top product

concentration would consist of the inert solvent (toluene and n-heptane). If Eqs. 4.82 and 4.83 are written in terms of the principal operating variables, we obtain the following:

$$\frac{\langle y_{T_2} \rangle_n}{y_o} = \left(\frac{P_T}{1 + P_B} \right)^{2n-2} \quad (4.84)$$

and

$$\frac{\langle y_{T_1} \rangle_n}{y_o} = \left(\frac{P_T}{1 + P_B} \right)^{2n-1} \quad (4.85)$$

There are certain values of P_T and P_B for which Eq. 4.83 is no longer true. When operating the parapump with $P_T < P_B$, the strongly adsorbed solute does not appear in the top product at steady state and Eq. 4.83 holds true. This situation is depicted in Fig. 4.9. The steady state characteristics are shown in Fig. 4.10 for the case in which $P_T < P_B$ and thus $L_i(T_1)/L_i(T_2) < 1$. In Fig. 4.10, by geometry, the bottom product concentration transients $\langle y_{B_1} \rangle_n$ can be derived as follows:

$$\frac{\overline{AB}}{\overline{AD}} = \frac{L_i(T_1)}{L_i(T_2)} = \left(\frac{1 + P_T + P_B}{1 + P_B} \right) \left(\frac{1 - b_i}{1 + b_i} \right) \quad (4.86)$$

Let

$$P_1 = \text{integer} \left[\frac{h - L_i(T_1)}{L_i(T_2) - L_i(T_1)} \right] \quad (4.87)$$

and

$$\begin{aligned} r_1 &= P_1 + 1 \\ &= \text{number of cycles necessary for the establishment of} \\ &\quad \text{steady state characteristic pattern.} \end{aligned}$$

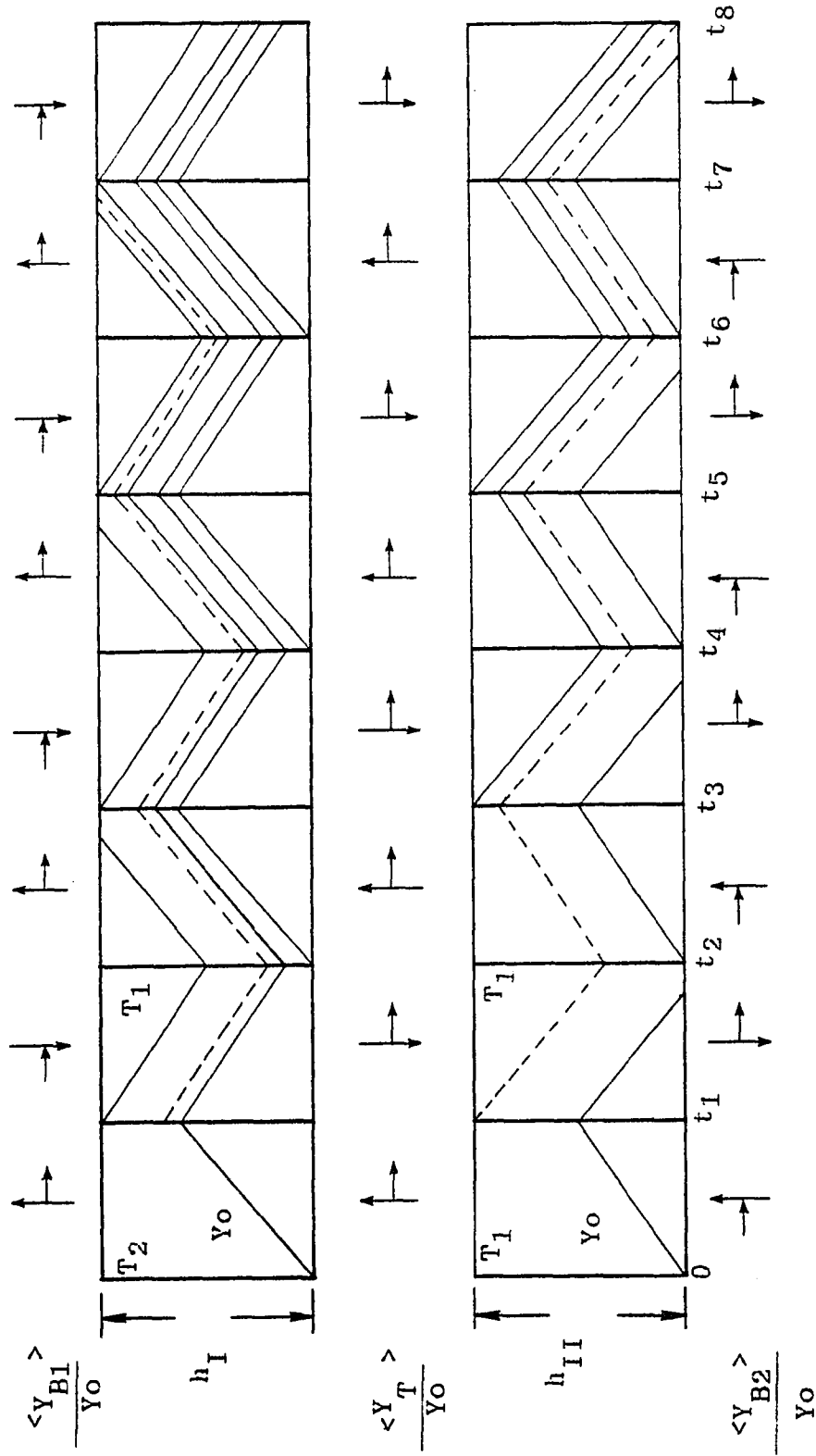


FIGURE 4.9 NET MOVEMENT OF CONCENTRATION FRONTS OF THE STRONGLY ADSORBED COMPONENT FOR A PSEUDO-BINARY SYSTEM WHERE $L_i(T_1)/L_i(T_2) < 1$

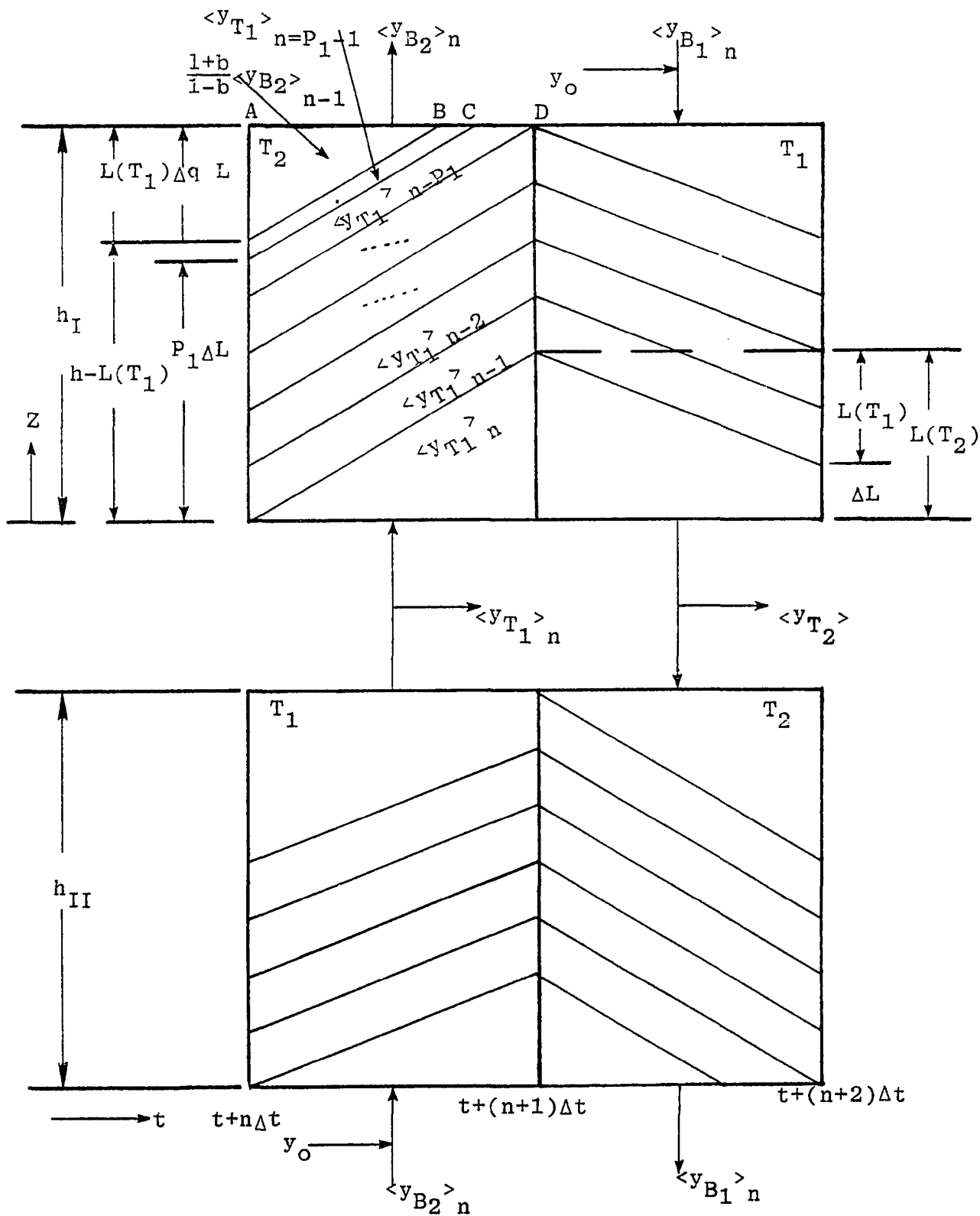


FIGURE 4.10:
STEADY STATE CHARACTERISTICS FOR THE STRONGLY ADSORBED COMPONENT
FOR A PSEUDO-BINARY SYSTEM, $L(T_1)/L(T_2) < 1$

Where

$$P_1 + q_1 = \frac{h - L_i(T_1)}{L_i(T_2) - L_i(T_1)} = \frac{h - L_i(T_1)}{\Delta L_i} \quad (4.88)$$

$P_1 =$ zero or a positive integer

and

$$0 \leq q_1 \leq 1$$

Therefore,

$$\frac{\overline{BC}}{q_1 \Delta L_i} = \frac{\Delta t}{L_i(T_2)} \quad (4.89)$$

or

$$\frac{\overline{BC}}{\overline{AD}} = \frac{\overline{BC}}{\Delta t} = \frac{q_1}{L_i(T_2)} \Delta L_i \quad (4.90)$$

$$= \left[\frac{L_i(T_2) - L_i(T_1)}{L_i(T_2)} \right] q_1$$

$$= \left[1 - \frac{L_i(T_1)}{L_i(T_2)} \right] q_1$$

$$\frac{\overline{CD}}{\overline{AD}} = 1 - \frac{\overline{AC}}{\overline{AD}}$$

$$= 1 - \left[\frac{L_i(T_1)}{L_i(T_2)} + \left(1 - \frac{L_i(T_1)}{L_i(T_2)} \right) q_1 \right] \quad (4.91)$$

Therefore, the bottom product concentration after n th cycle can then be calculated from the following (see Fig. 4.10)

$$\langle y_{B1} \rangle_n = \left(\frac{1 + b_i}{1 - b_i} \right) \frac{\overline{AB}}{\overline{AD}} \langle y_{B2} \rangle_{n-1} + \frac{\overline{BC}}{\overline{AD}} \langle y_{T1} \rangle_{n-P_1} - 1 + \frac{\overline{CD}}{\overline{AD}} \langle y_{T1} \rangle_{n-P_1} \quad (4.92)$$

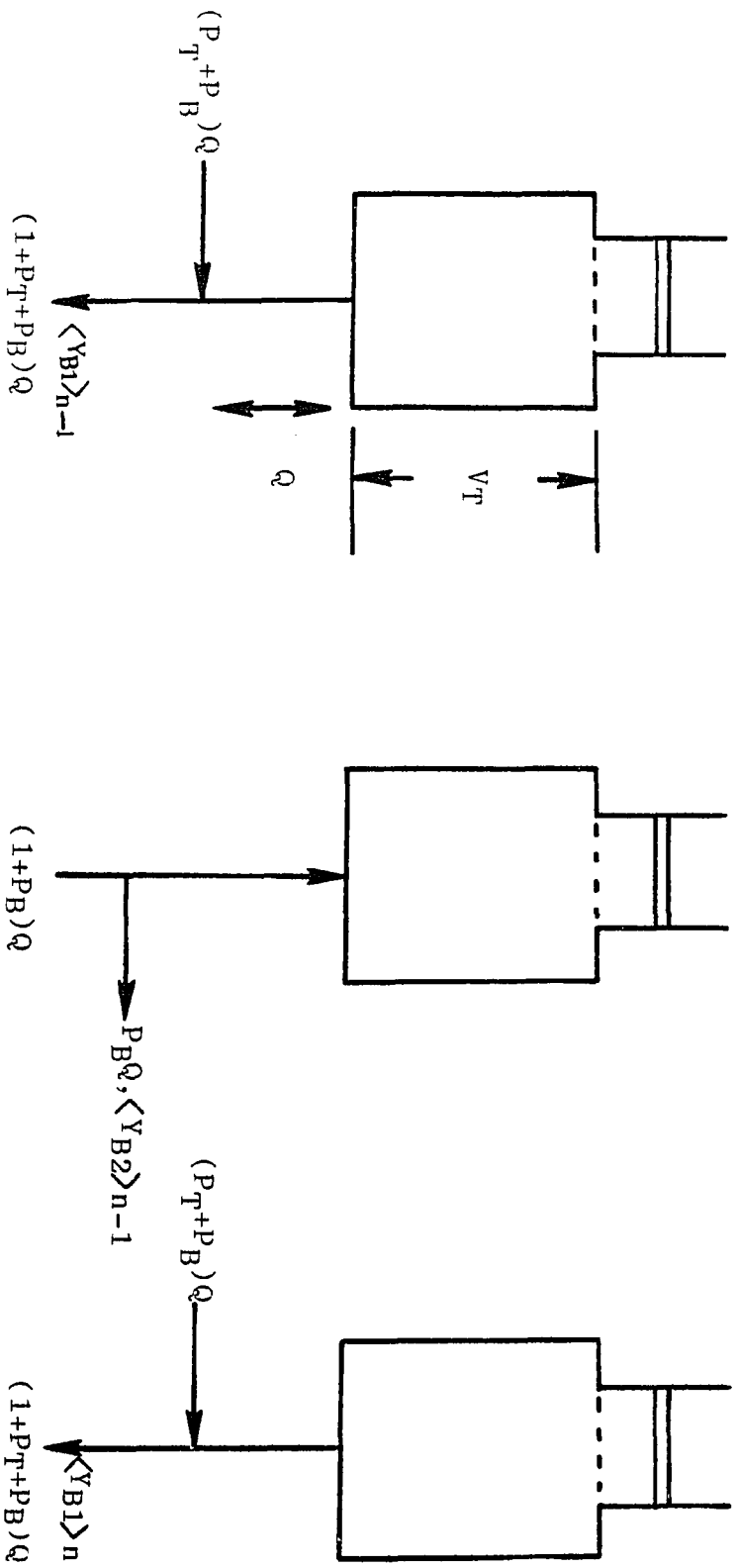


FIGURE 4.11 TOP COLUMN EXTERNALS FOR TWO COLUMN PARAMETRIC PUMP WITH ALTERNATING TOP FEED

And upon substitution of Eqs. 4.86, 4.90 and 4.91 into Eq. 4.92 the following is obtained

$$\langle y_{B1} \rangle_n = \frac{1 - b_i}{1 + b_i} \langle y_{B2} \rangle_{n-1} + \left(1 - \frac{L_i(T_2)}{L_i(T_1)}\right) q_1 \left[\langle y_{T1} \rangle_{n-p-1} + (1-q_1) \langle y_{T1} \rangle_{n-p_i} \right] \quad (4.93)$$

For the case in which $P_B \geq P_T$ or $L_i(T_1)/L_i(T_2) \geq 1$, the steady state characteristics developed with these conditions result in incomplete separation, i.e. component B (more strongly adsorbed component) is found in the product taken from the middle of the two columns ($\langle y_{T1} \rangle_n$). From experimental observations, the concentration increases as the magnitude of $L_i(T_1)/L_i(T_2)$ increases. In Figs. 4.12 and 4.13, by geometry, the concentration transients $\langle y_{T1} \rangle_n$ can be derived as follows:

$$\frac{\bar{EG}}{\bar{EF}} = \frac{L_i(T_2)}{L_i(T_1)} = \left(\frac{1 + P_B}{1 + P_T + P_B} \right) \left(\frac{1 + b_i}{1 - b_i} \right) \quad (4.94)$$

$$P_2 = \text{integer} \left[\frac{h - L_i(T_2)}{L_i(T_1) - L_i(T_2)} \right]$$

$$P_2 + q_2 = \frac{h - L_i(T_2)}{L_i(T_1) - L_i(T_2)} = \frac{h - L_i(T_2)}{\Delta L_i}$$

Where

$$q_2 = \text{zero or a positive integer}$$

and

$$0 \leq q_2 \leq 1$$

Therefore

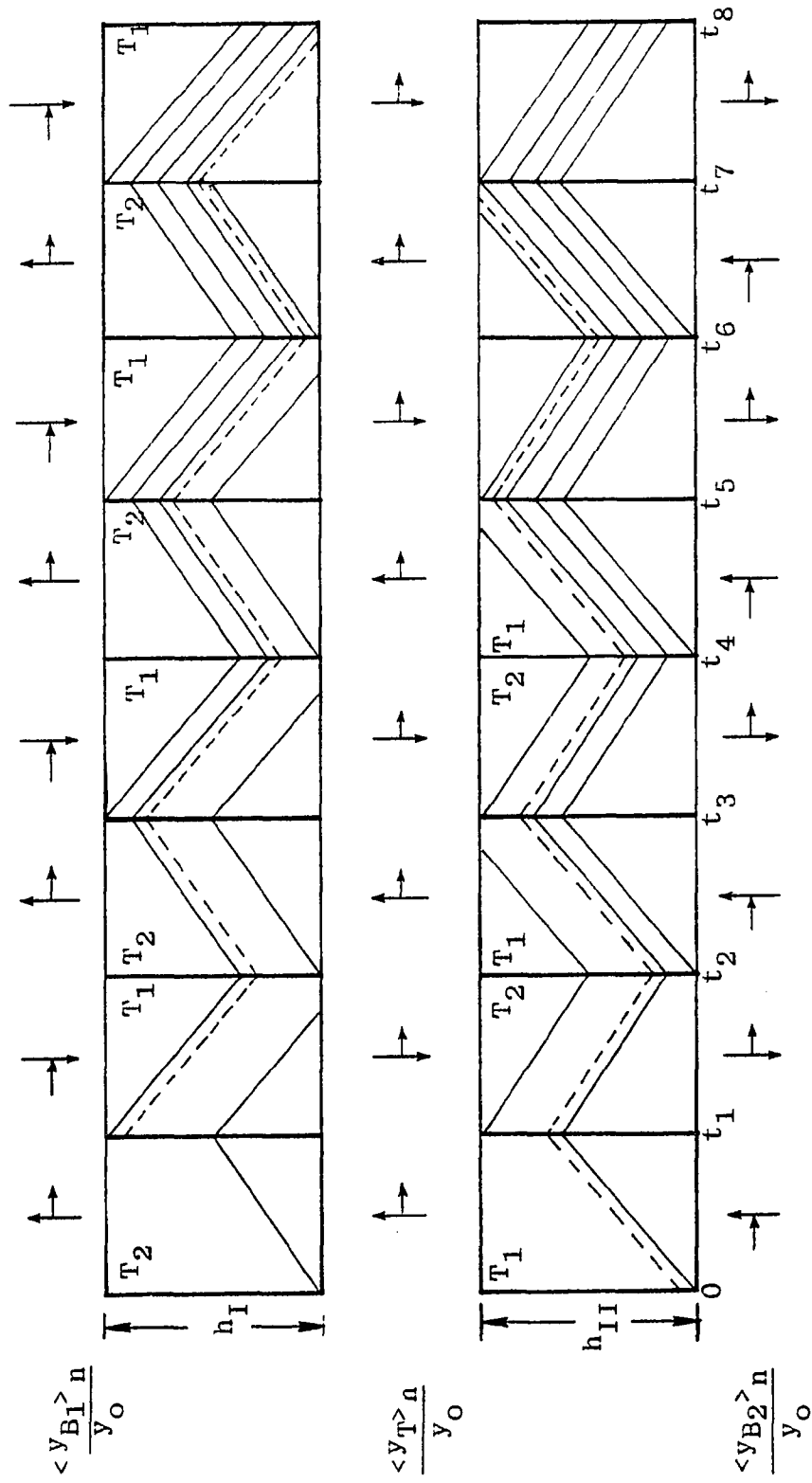


FIGURE 4.12 NET MOVEMENT OF CONCENTRATION FRONTS OF THE STRONGLY ADSORBED COMPONENT FOR A PSEUDO-BINARY SYSTEM WHERE $\frac{Li(T_1)}{Li(T_2)} > 1$

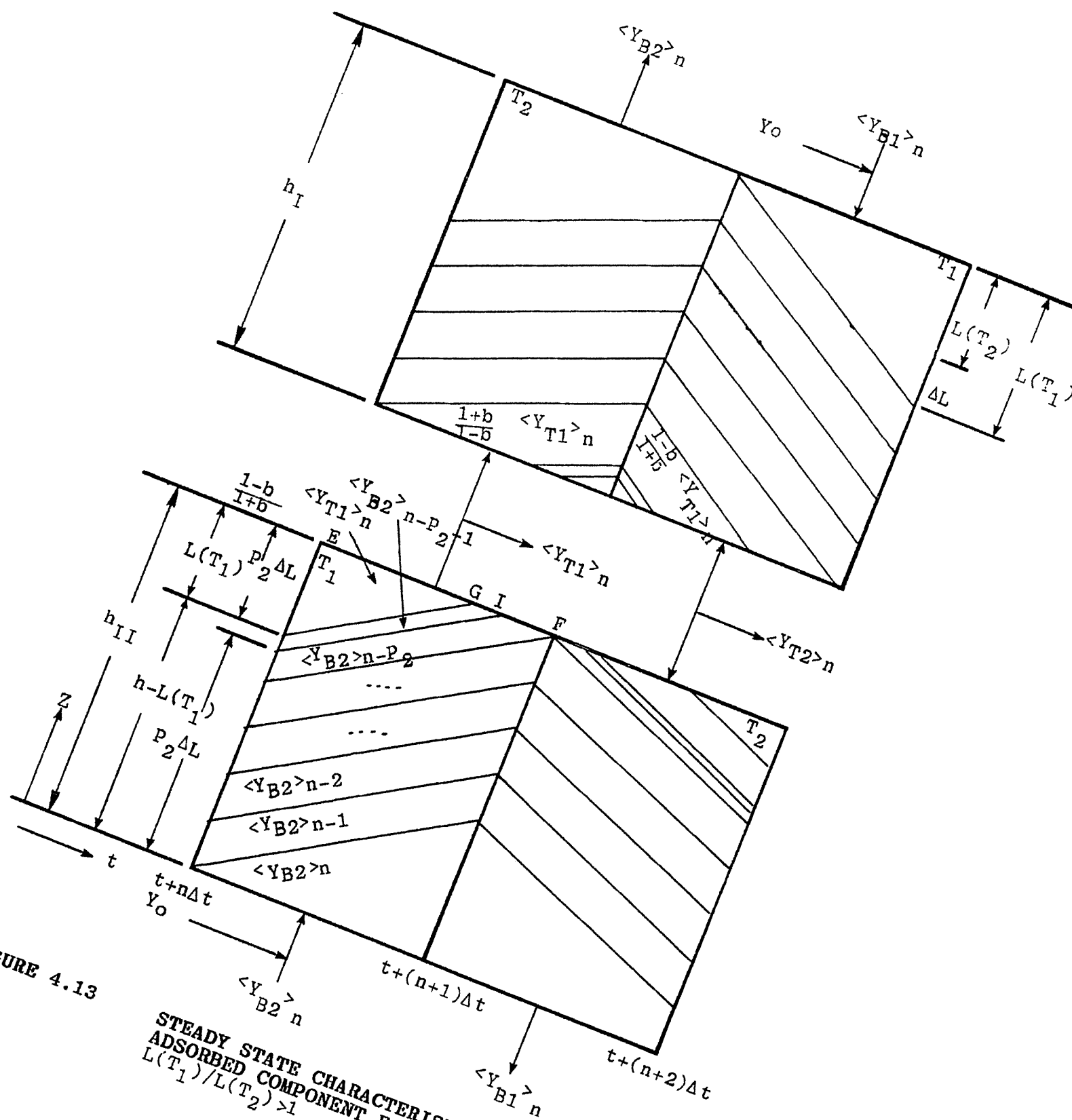


FIGURE 4.13

STEADY STATE CHARACTERISTICS FOR THE STRONGLY ADSORBED COMPONENT FOR A PSEUDO-BINARY SYSTEM, $L(T_1)/L(T_2) > 1$

$$\frac{\overline{GI}}{\overline{EF}} = \frac{\overline{GI}}{\Delta t} = \frac{q_2 \Delta L_i}{L_i(T_1)} = q_2 \left[\frac{L_i(T_1) - L_i(T_2)}{L_i(T_1)} \right] \quad (4.95)$$

$$\begin{aligned} \frac{\overline{IF}}{\overline{EF}} &= 1 - \frac{\overline{EI}}{\overline{EF}} \\ &= 1 - \left[\frac{L_i(T_2)}{L_i(T_1)} + q_2 \left(1 - \frac{L_i(T_2)}{L_i(T_1)} \right) \right] \\ &= \left(1 - \frac{L_i(T_2)}{L_i(T_1)} \right) (1 - q_2) \end{aligned} \quad (4.96)$$

Therefore the top product, $\langle y_{T1} \rangle_n$, concentration after nth cycle can then be calculated from

$$\langle y_{T1} \rangle_n = \langle y_{T1} \rangle_n \left(\frac{1-b}{1+b} \right) \frac{\overline{EG}}{\overline{EF}} + \langle y_{B2} \rangle_{n-P_2-1} \frac{\overline{GI}}{\overline{EF}} + \langle y_{B2} \rangle_{n-P_2} \frac{\overline{IF}}{\overline{EF}} \quad (4.97)$$

Upon substitution of Eqs. 4.94 through 4.96 into Eq. 4.97, we obtain

$$\langle y_{T1} \rangle_n = \frac{1-b}{1+b} \langle y_{T2} \rangle_n + \left(1 - \frac{L_i(T_2)}{L_i(T_1)} \right) \left[q_2 \langle y_{B2} \rangle_{n-P_2-1} + (1 - q_2) \langle y_{B2} \rangle_{n-P_2} \right] \quad (4.98)$$

The bottom product concentration $\langle y_{B1} \rangle_n$ can also be calculated by making a solute and total mass balance.

Staged Sequence Adsorption Process

Figure 4.14 shows the column arrangement for the staged sequence adsorption process. The interstitial velocities, ev , of the material in the three columns for stage 1 are,

$$h_I: \quad (R + P_T + P_I)Q = (R + P_T + P_I)v_OA \quad (4.99)$$

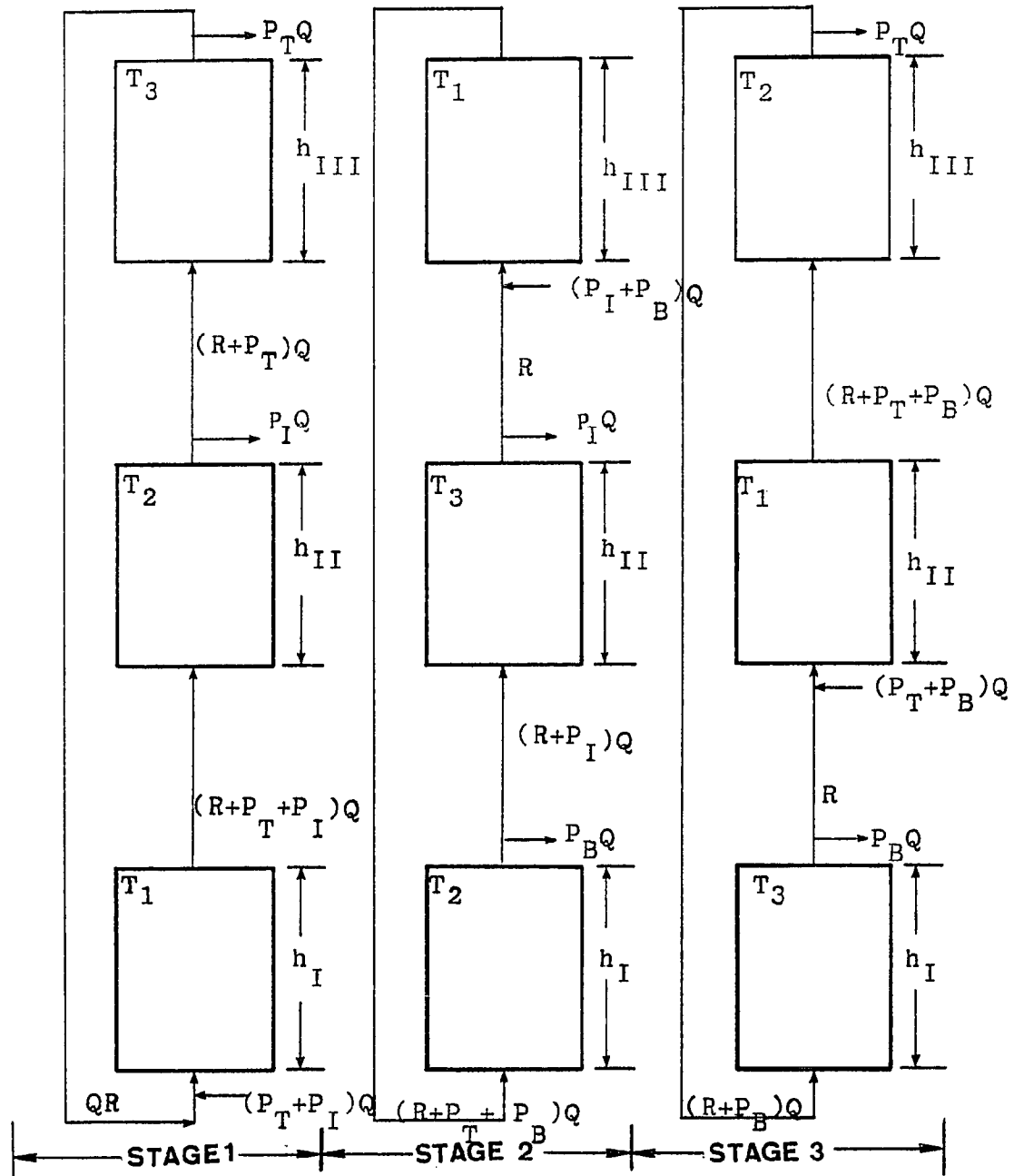


FIGURE 4.14:
COLUMN ARRANGEMENT FOR STAGED SEQUENCE CYCLIC PROCESS

$$h_{II}: (R + P_T + P_I)Q = (R + P_T + P_I)v_0A \quad (4.100)$$

$$h_{III}: (R + P_T)Q = (R + P_T)v_0A \quad (4.101)$$

where

R = amount of material refluxed in ml.

The slopes of the characteristics can then be written in terms of Eqs. 4.99 to 4.101 and Eqs. 4.54 and 4.55

$$\text{Column I: } u_{i,\text{con}} \equiv \left(\frac{\partial z}{\partial t}\right)_{T_1} = \frac{(R + P_T + P_I)v_0}{(1 + b^3_i)[1 + 0.5(m_i(T_1) + m_i(T_3))]} \quad (4.102)$$

$$\text{Column II: } u_{i,\text{con}} \equiv \left(\frac{\partial z}{\partial t}\right)_{T_2} = \frac{(R + P_T + P_I)v_0}{(1 - b^1_i)[1 + 0.5(m_i(T_1) + m_i(T_2))]} \quad (4.103)$$

$$\text{Column III: } u_{i,\text{con}} \equiv \left(\frac{\partial z}{\partial t}\right)_{T_3} = \frac{(R + P_T)v_0}{(1 - b^2_i)[1 + 0.5(m_i(T_2) + m_i(T_3))]} \quad (4.104)$$

Upon integration of Eqs. 4.102 to 4.104, between the limits of $t = t_1$ and $t = t_2$, we get the wave front penetration distances for the stage 1 mode of operation.

$$L_i(T_1) = \frac{(R + P_T + P_I)v_0}{(1 + b^3_i)[1 + 0.5(m_i(T_1) + m_i(T_3))]} \cdot \Delta t \quad (4.105)$$

$$L_i(T_2) = \frac{(R + P_T + P_I)v_0}{(1 - b^1_i)[1 + 0.5(m_i(T_1) + m_i(T_3))]} \cdot \Delta t \quad (4.106)$$

$$L_i(T_3) = \frac{(R + P_T)v_0}{(1 - b_i^2)[1 + 0.5(m_i(T_2) + m_i(T_3))]} \cdot \Delta \quad (4.107)$$

Figures 4.15 and 4.16 illustrate the concentration characteristics for two solute systems assuming linear isotherms. Figure 4.15 illustrates a case with the penetration distances for the two components equal $L_A(T_1)=0.33h$, $L_A(T_2)=0.50h$, $L_A(T_3)=0.66h$; $L_B(T_1)=0.166h$, $L_B(T_2) = 0.33h$ and $L_B(T_3)=0.50h$, where h is the height of the column. It is assumed that $h_I=h_{II}=h_{III}$. Some of the concentration wave fronts originating from T_1 do not break through the column after experiencing a sequence of three temperature inputs. As a consequence, component A peaks at T_3 instead of T_2 and component B concentrates at the temperature boundary. Baker and Pigford (1971) noted that by adjusting the thermal velocity and thus the penetration distance of the thermal wave to override the natural thermal wave, certain concentration wave fronts can be amplified. By so doing, of course, the concentration waves can be made to concentrate at desired points between two given temperature boundaries. This lag in concentration waves can also be directed to exit or emerge at desired points within a given temperature if the frequencies of the temperature inputs are varied (i.e. if the duration of the stages are made nonsymmetrical). As predicted by equilibrium theory, the concentration characteristics will change according to Eq. 4.70 or

$$\frac{y(T_1)}{y(T_2)} = \frac{1 - b_i^1}{1 + b_i^3} \quad (4.108)$$

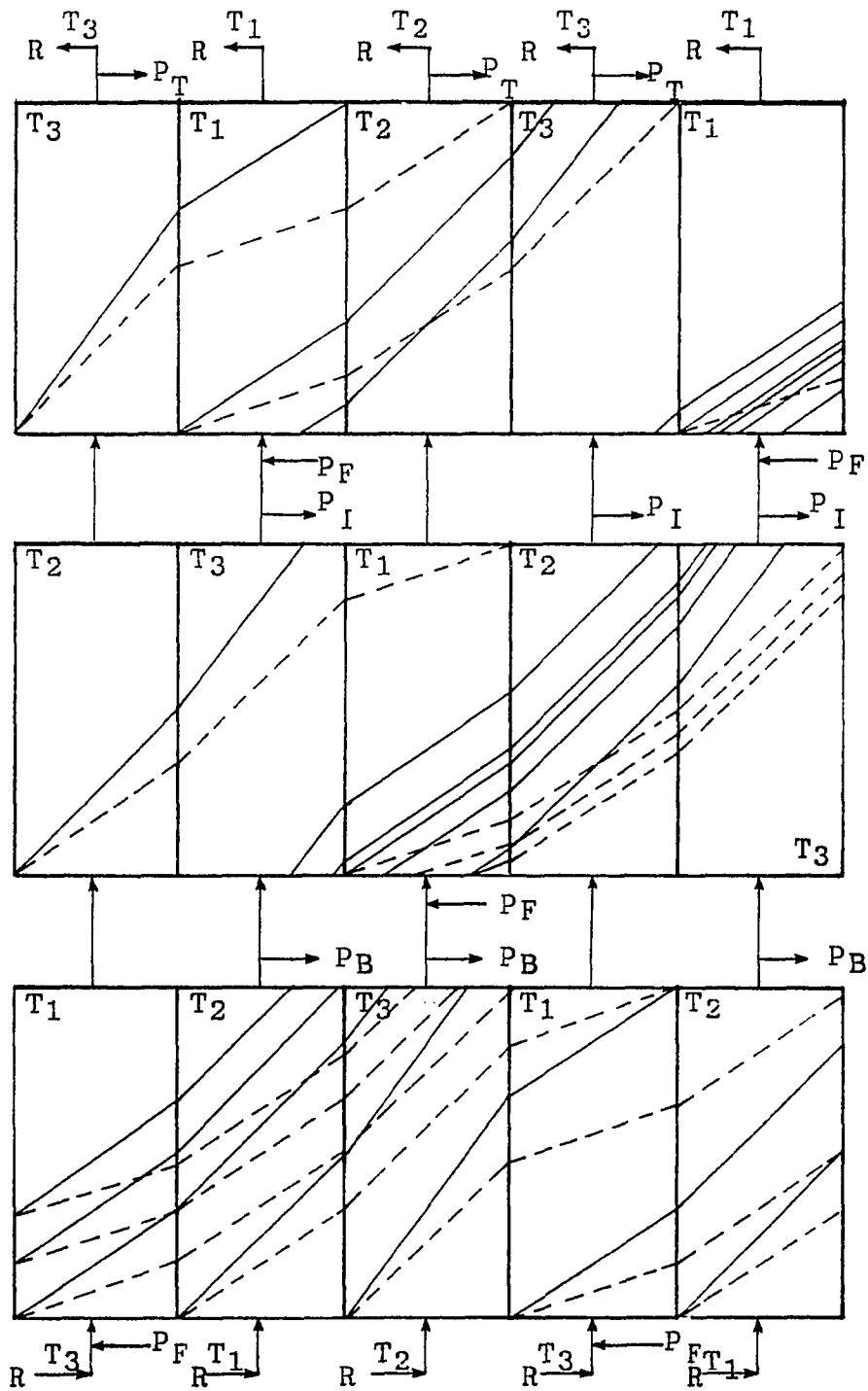


FIG.4.15 : CONCENTRATION WAVE FRONTS FOR STAGED SEQUENCE CYCLIC PROCESS

$$L_A(T_1) = 0.33h, \quad L_A(T_2) = 0.50h, \quad L_A(T_3) = 0.66h;$$

$$L_B(T_1) = 0.166h, \quad L_B(T_2) = 0.33h \quad \text{and} \quad L_B(T_3) = 0.50h$$

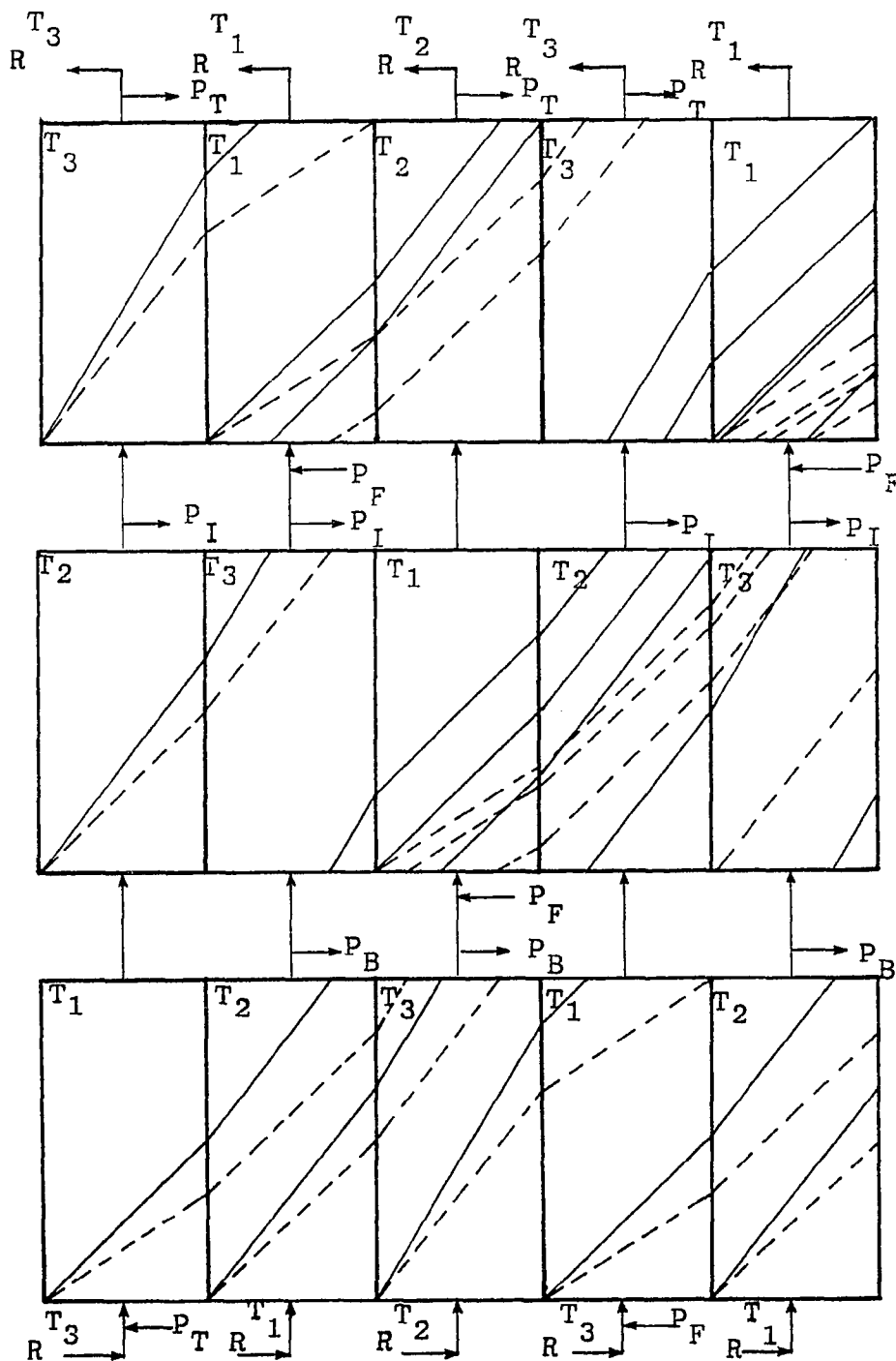


FIGURE 4.16:
CONCENTRATION WAVE FRONTS FOR STAGED SEQUENCE CYCLIC PROCESS
 $L_A(T_1) = 0.5h$, $L_A(T_2) = 0.66h$, $L_A(T_3) = 0.833h$;
 $L_B(T_1) = 0.33h$, $L_B(T_2) = 0.5h$ and $L_B(T_3) = 0.66h$

and

$$\frac{y(T_2)}{y(T_3)} = \frac{1 - b_i^2}{1 - b_i^1} \quad (4.109)$$

Figure 4.16 illustrates a case where component A has been directed to exit the column at T_2 and component B at T_3 . For this case, the penetration distances for the two components are $L_A(T_1)=0.5h$, $L_A(T_2)=0.66h$, $L_A(T_3)=0.833h$; $L_B(T_1)=0.33h$, $L_B(T_2)=0.5h$ and $L_B(T_3)=0.66h$. Some of the characteristic wave fronts of component A ($L_A(T)$ $L_B(T)$) originating from a column at T_1 only see a change in temperature once (T_2) before exiting, while component B originating from the same source see T_2 and T_3 before exiting. With proper selection of operating conditions such as P_T , P_B and P_I and for the most part v_O , the concentration characteristics can be made to undergo a series of temperature changes, thereby building concentrated characteristic wave fronts before exiting.

CHAPTER 5

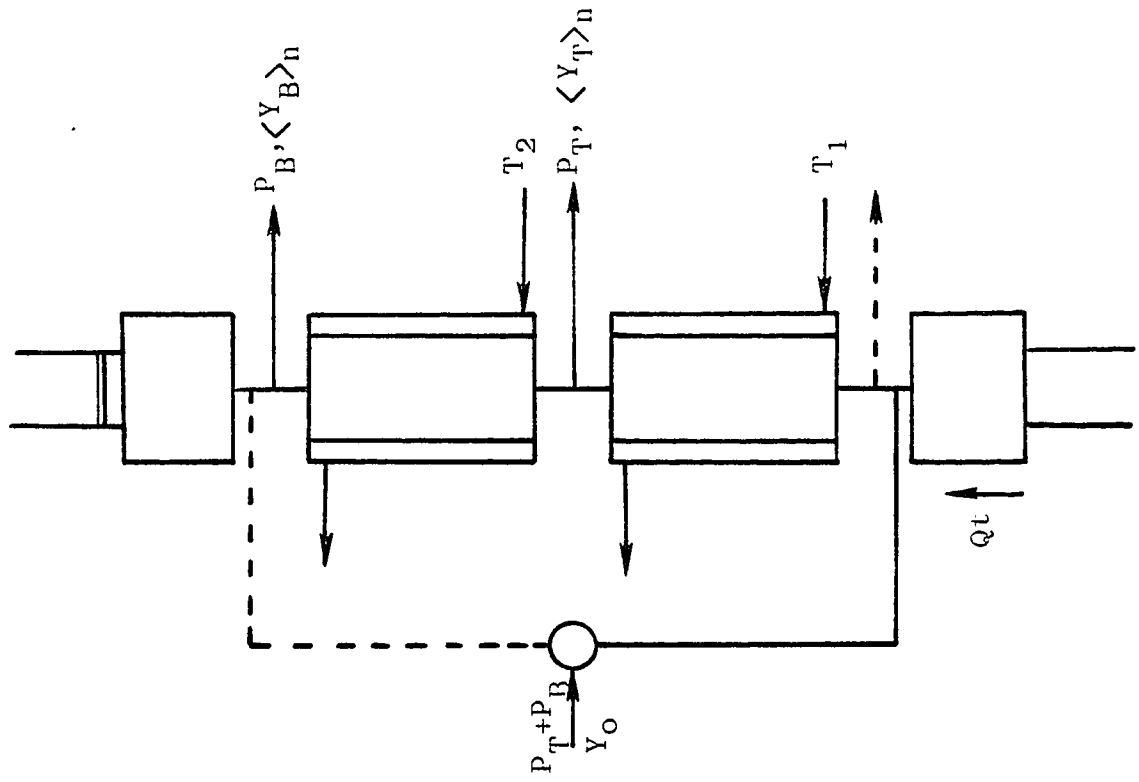
SEPARATION OF DILUTE MULTICOMPONENT SOLUTIONS BY CYCLIC ADSORPTION AND PARAMETRIC PUMPING

The cyclic adsorption process and parametric pumping are operated continuously. They are continuous in the sense that the feed is steadily introduced and the products continuously withdrawn.

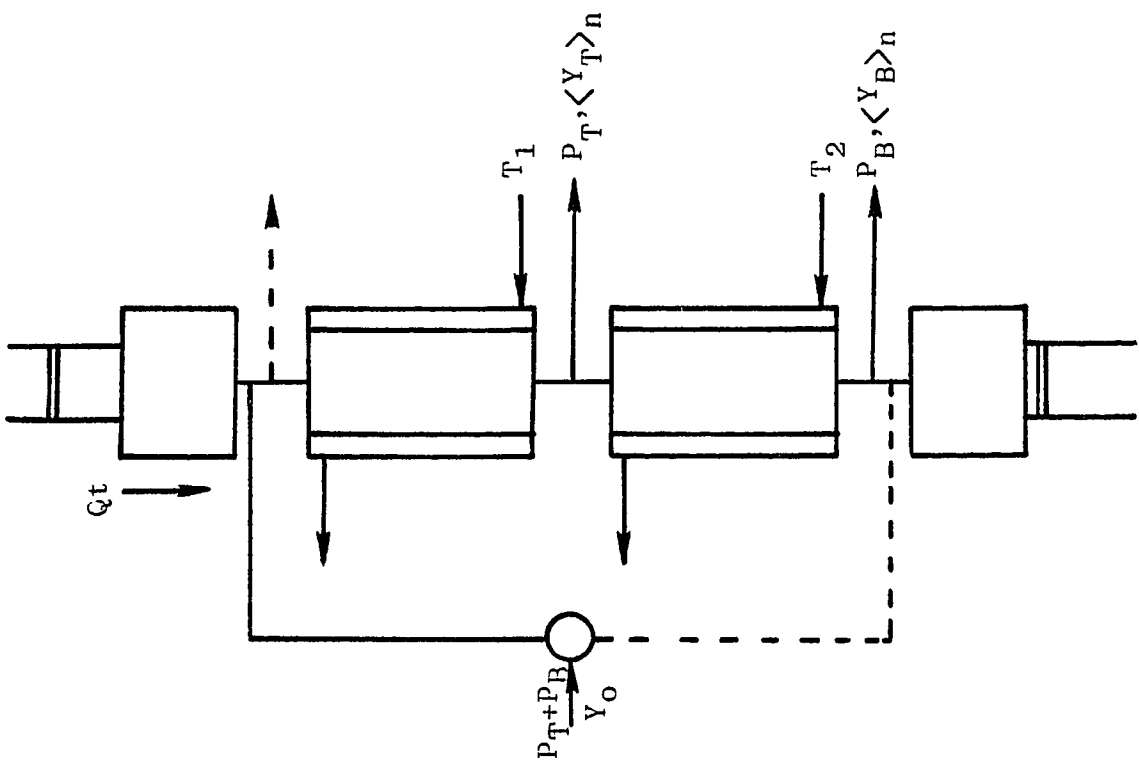
SEPARATION BY PARAMETRIC PUMPING

Figure 5.1 illustrates the schematics of the column arrangement for the downflow first half cycle and the upflow second half cycle. The flowrate to and from the reservoirs of the parapump during each half cycle is Q (volume-units per unit time). The duration time of each half cycle is t (time units), therefore the displacement volume is Qt . The dead volumes associated with the top and bottom reservoirs are V_T and V_B respectively.

The feed flow rate is $Q(P_T+P_B)$ and the top and bottom product flow rates are QP_T and QP_B , respectively, where P_T and P_B are the ratios of the top and bottom product flow rates to the reservoir displacement rate. The feed stream during the first half cycle is located at the top of column I (Fig. 5.1-a) and at the bottom of column II (Fig. 5.1-b) during the second half cycle. The feed and product streams flow steadily during the upflow and downflow half cycles. The column internal flow rates can easily be obtained from the flow diagrams as shown in Fig. 6.1. The external material balances could be made around the points of



(b)



(a)

FIGURE 5.1 SCHEMATIC OF A TWO COLUMN PARAMETRIC PUMP WITH ALTERNATING TOP FEED

bottom and top product withdrawal. During downflow, the flow rate in column I is $(1+P_T+P_B)Q$, and in column II is $(1+P_B)Q$, while the upflow flow rate in column I is $(1+P_B)Q$ and that of column II is $(1+P_T+P_B)Q$. The given product streams during discharge come only from the column and not from the reservoir, nor from the feed stream.

At the start of the run, the column is filled with adsorbent particles, the column voids and the reservoirs are filled with a three-component mixture, two components of which distribute between the two phases. Column I is at temperature T_1 and column II at temperature T_2 during downflow, while column I is at temperature T_2 and column II is at temperature T_1 during upflow. The material from the reservoir and feed are assumed to be well mixed before they are fed to the column. The volume of material in the connecting lines is assumed to be included in the dead volume of the adjacent reservoir. Before the parapumping operation is started, the distribution of solutes in the fluid phase is equal to the feed concentration y_0 throughout the apparatus and they are equilibrated with the solute concentration on the adsorbent particles at the higher temperature T_2 . The pumping operation is started by changing the temperature of column I from T_2 to T_1 and maintaining column 2 at T_1 coupled with downward flow.

The parametric pumping parameters just in the on-going analysis are used in the mathematical development of the adsorption-desorption of the fluid mixtures in the column during the parametric pumping operation, and the flow processes occurring

within the column (internal equations). External equations, which are also necessary, are the solute material balances on streams flowing to and from a reservoir which also consider the feed and product streams.

Internal Equations

For the analysis of the internal equations, the equilibrium theory of Pigford et al. (1969) will be used. The equilibrium theory was originated by Pigford (1969) and generalized by Aris (1969), and extended to continuous direct mode parametric pumping by Chen and Hill (1971) and Chen et al. (1972), and also applied to the analysis of cycling zone adsorption by Baker and Pigford (1971), Gupta and Sweed (1971) and Wankat (1971). The following assumptions were made:

1. interphase equilibrium is established at any point in the bed;
2. a linear distribution law which has a temperature-dependent distribution coefficient exists;
3. rate of heat transfer is high, therefore temperature change within the column is instantaneous;
4. steady unidirectional flow of all fluid elements (plug flow);
5. axial dispersion is negligible;
6. change of fluid density is negligible (total moles of fluid per unit volume of fluid, and total moles of fluid per unit volume of solid are constant). In the

equations, the terms y_i and x_i incorporate the fluid density, ρ_f , and solid density, ρ_s , terms shown by Pigford et al. (1969).

Based on the above simplifying assumptions, the solute material balance in both the fluid and solid phase is:

$$\epsilon \frac{\partial y_i}{\partial t} + \epsilon v \frac{\partial y_i}{\partial z} + (1 - \epsilon) \frac{\partial x_i}{\partial t} = 0 \quad (5.1)$$

Subject to the linear equilibrium isotherm,

$$x_i = M_i(T)y_i \quad (5.2)$$

If the linear isotherm is differentiated

$$\frac{\partial x_i}{\partial t} = M_i(T) \frac{\partial y_i}{\partial t} + y_i \frac{\partial M_i(T)}{\partial T} \cdot \frac{\partial T}{\partial t} \quad (5.3)$$

if

$$m_i = \frac{(1 - \epsilon)}{\epsilon} M_i(T) \quad (5.4)$$

Then

$$\frac{\partial m_i}{\partial T} = \frac{(1 - \epsilon)}{\epsilon} \frac{\partial M_i(T)}{\partial T} \quad (5.5)$$

By substitution, Eq. 5.1 becomes

$$(1 + m_i) \frac{\partial y_i}{\partial t} + v \frac{\partial y_i}{\partial z} + \frac{\partial m_i}{\partial T} \cdot \frac{\partial T}{\partial t} \cdot y_i = 0 \quad (5.6)$$

By the method of characteristics, we get

$$\frac{dt}{1 + m_i} = \frac{dz}{v} = \frac{-dy_i}{\frac{dm_i}{dT} \cdot \frac{dT}{dt} \cdot y_i} \quad (5.7)$$

which beomes

$$\frac{dz}{dt} = \frac{v}{1 + m_i} = u_{con} = \frac{v}{1 + \frac{(1 - \epsilon)}{\epsilon} M_i(T)} \quad (5.8)$$

TABLE 5.1
Two Column Continuous Parametric Pumping Characteristics

	Column Flowrate		Product Flow Rate Limits	$\frac{L_i(T_1)}{v\Delta t}$	$\frac{L_i(T_2)}{v\Delta t}$
	Downflow	Upflow			
Column I	$(1+P_T+P_B)Q$	$(1+P_B)Q$	$P_T \leq 0.3$ $P_B \geq 0.1$	$-\left[\frac{1+P_T+P_B}{1+\left(\frac{1-\epsilon}{\epsilon}\right)M_i(T_1)} \right]$	$+\left[\frac{1+P_B}{1+\left(\frac{1-\epsilon}{\epsilon}\right)M_i(T_2)} \right]$
Column II	$(1+P_B)Q$	$(1+P_T+P_B)Q$	$P_T < 0.3$ $P_B \geq 0.3$	$-\left[\frac{1+P_T+P_B}{1+\left(\frac{1-\epsilon}{\epsilon}\right)M_i(T_1)} \right]$	$+\left[\frac{1+P_B}{1+\left(\frac{1-\epsilon}{\epsilon}\right)M_i(T_2)} \right]$
	Penetration Distance Inequalities		Loci of Switching Points		
	Downflow	Upflow	Downflow	Upflow	
Column I	$L_A(T_1) > H_{col}$ $L_B(T_1) \leq H_{col}$	$L_A(T_2) < H_{col}$ $L_B(T_2) > H_{col}$	$L_B(T_1) < H_{col}$	$L_B(T_2) > H_{col}$	
Column II	$L_A(T_2) < H_{col}$ $L_B(T_2) > H_{col}$	$L_A(T_1) > H_{col}$ $L_B(T_1) \leq H_{col}$	$L_B(T_2) > H_{col}$	$L_B(T_1) < H_{col}$	

Meaning that in the z-t plane, the characteristic curves are straight lines having slopes of u_{con} . If Eq. 5.8 is integrated between the limits of $t=t_a$ and $t=t_b$, we get the wave front penetration distances for hot upflow and cold downflow, respectively (the concept of which was first defined by Chen and Hill [1971]).

$$L_i(T) = u_{con} t = \frac{v}{1 + \frac{(1 - \epsilon)}{\epsilon} M_i(T)} \Delta t \quad (5.9)$$

Now, from Figure 5.2 and Table 5.1, the flow rates in the columns during the downflow are Column I ($= (1+P_T+P_B)Q$) and Column II ($= (1+P_B)Q$); and during the upflow, Column I ($= (1+P_B)Q$) and Column II ($= (1+P_T+P_B)Q$) and Eq. 5.9 becomes:

Downflow:

$$L_i^I(T_1) = - \left[\frac{v(1 + P_T + P_B)\Delta t_1}{1 + \left(\frac{1 - \epsilon}{\epsilon}\right)M_i(T_1)} \right] \quad (5.10)$$

$$L_i^{II}(T_2) = - \left[\frac{v(1 + P_B)\Delta t_1}{1 + \left(\frac{1 - \epsilon}{\epsilon}\right)M_i(T_2)} \right] \quad (5.11)$$

Upflow:

$$L_i^I(T_2) = + \left[\frac{v(1 + P_B)\Delta t_2}{1 + \left(\frac{1 - \epsilon}{\epsilon}\right)M_i(T_2)} \right] \quad (5.12)$$

$$L_i^{II}(T_1) = + \left[\frac{v(1+P_T + P_B)\Delta t_2}{1 + \left(\frac{1 - \epsilon}{\epsilon}\right)M_i(T_1)} \right] \quad (5.13)$$

while the negative and positive signs indicate the downflow and upflow directions respectively.

For component A, where $M_A(T) < M_B(T)$ and therefore $L_A(T) > L_B(T)$,

$$\frac{L^I_A(T_1)}{L^I_A(T_2)} = \left[\frac{v(1 + P_T + P_B)\Delta t_1}{1 + \left(\frac{1 - \epsilon}{\epsilon}\right)M_A(T_1)} \right] \cdot \left[\frac{1 + \left(\frac{1 - \epsilon}{\epsilon}\right)M_A(T_2)}{v(1 + P_B)\Delta t_2} \right] \quad (5.14)$$

$$= \left[\frac{1 + P_T + P_B}{1 + P_B} \right] \cdot \left[\frac{\epsilon + (1 - \epsilon)M^I_A(T_2)}{\epsilon + (1 - \epsilon)M^I_A(T_1)} \right] \cdot \left[\frac{\Delta t_1}{\Delta t_2} \right] \quad (5.15)$$

As shown by Chen and Hill (1971), one can also conclude that the degree of purity of A in the top by parametric pumping depends on the relative magnitudes of $L^I_A(T_1)/L^I_A(T_2)$ and the height of column I, H^I . To be able to have most of B in the bottom product,

$$\frac{L^I_B(T_1)}{L^I_B(T_2)} = \left[\frac{1 + P_T + P_B}{1 + P_B} \right] \cdot \left[\frac{\epsilon + (1 - \epsilon)M^I_B(T_2)}{\epsilon + (1 - \epsilon)M^I_B(T_1)} \right] \cdot \left[\frac{\Delta t_1}{\Delta t_2} \right] \quad (5.16)$$

Which also depends on the relative magnitudes of $L^I_B(T_1)/L^I_B(T_2)$ and the height of column I, H^I . Following the same reasoning, to be able to have most of component A and B in the top and bottom product respectively in column II, the following relative magnitude of penetration distances holds:

$$\frac{L^{II}_A(T_2)}{L^{II}_A(T_1)} = \left[\frac{1 + P_B}{1 + P_T + P_B} \right] \cdot \left[\frac{\epsilon + (1 - \epsilon)M^{II}_A(T_2)}{\epsilon + (1 - \epsilon)M^{II}_A(T_1)} \right] \cdot \left[\frac{\Delta t_1}{\Delta t_2} \right] \quad (5.17)$$

and

$$\frac{L^{II}_B(T_2)}{L^{II}_B(T_1)} = \left[\frac{1 + P_B}{1 + P_T + P_B} \right] \cdot \left[\frac{\epsilon + (1 - \epsilon)M^{II}_B(T_2)}{\epsilon + (1 - \epsilon)M^{II}_B(T_1)} \right] \cdot \left[\frac{\Delta t_1}{\Delta t_2} \right] \quad (5.18)$$

In order to direct the movement of component A to the top product and component B to the bottom product, the following inequalities must be satisfied:

$$\frac{L_A^I(T_1)}{L_A^I(T_2)} > 1 \quad \text{and} \quad L_A^I(T_1) > H_{col}^I \quad (5.19)$$

$$\frac{L_B^I(T_1)}{L_B^I(T_2)} < 1 \quad \text{and} \quad L_B^I(T_1) < H_{col}^I \quad (5.20)$$

$$\frac{L_A^{II}(T_2)}{L_A^{II}(T_1)} < 1 \quad \text{and} \quad L_A^{II}(T_2) < H_{col}^{II} \quad (5.21)$$

$$\frac{L_B^{II}(T_2)}{L_B^{II}(T_1)} > 1 \quad \text{and} \quad L_B^{II}(T_2) < H_{col}^{II} \quad (5.22)$$

Equations 5.19 through 5.22 provide the necessary guidelines that must be satisfied for a satisfactory pump performance. From Equations 5.17 through 5.18, one can see that the relative magnitude of the penetration distances consists of three terms. The first term is the ratio of the flow rates in the columns during downflow to the flow rates during upflow. The second term is the ratio of the equilibrium capacity of each component at a given temperature, and the third term is the ratio of the duration time for each half cycle. For a given material, the equilibrium capacity of each component at a given temperature is fixed. The ratios of the flow rates and the half cycle duration time only provides the parapumper the means to get a desired ratio of the relative penetration distances for a given cycle and temperature. Since the bulk velocity of the pumping operation would be fixed for a given operation, the change in the ratios of the flow rates can be achieved by proper adjustment of

the size of products withdrawn from the top (P_T) and bottom (P_B). The half cycle time could be made symmetrical (the duration time for downflow half cycle equal to the duration time for upflow half cycle) or asymmetrical (the duration time for downflow half cycle not equal to the duration time for upflow half cycle). For all runs done in this study, symmetrical half cycle times were used.

By substituting Eq. 5.14 into Eq. 5.19, the following is obtained,

$$\left(\frac{1 + P_T + P_B}{1 + P_B}\right) \left(\frac{\epsilon + (1 - \epsilon)M_A^I(T_2)}{\epsilon + (1 - \epsilon)M_A^I(T_1)}\right) \frac{\Delta t_1}{\Delta t_2} > 1 \quad (5.23)$$

$$\frac{1 + P_T + P_B}{1 + P_B} > \frac{\Delta t_2}{\Delta t_1} \left[\frac{\epsilon + (1 - \epsilon)M_A^I(T_1)}{\epsilon + (1 - \epsilon)M_A^I(T_2)}\right] \quad (5.24)$$

Define

$$\Delta M_i^I = \left[\frac{\epsilon + (1 - \epsilon)M_i^I(T_{k,j-1})}{\epsilon + (1 - \epsilon)M_i^I(T_{k,j})}\right] \quad (5.25)$$

ΔM_i is the equilibrium capacity coefficient for component i where $T_{k,j-1}$ denotes the previous temperature at a given position k , and time interval $j-1$ at which the equilibrium coefficient is evaluated while $T_{k,j}$ is the new temperature at the same position k and new time interval j .

For symmetrical half cycle duration time, and upon rearrangement,

For component A,

$$\frac{P_T + P_B}{P_B} > \Delta M^I_A \quad (5.26)$$

$$\frac{P_E}{P_T + P_B} < \Delta M^{II}_A \quad (5.27)$$

For component B

$$\frac{P_T + P_B}{P_B} < \Delta M^I_B \quad (5.28)$$

and

$$\frac{P_B}{P_T + P_B} > \Delta M^{II}_B \quad (5.29)$$

For physical adsorption such as the phenomena normally found in separation of hydrocarbons, the right hand member of Eqs. 5.26 through 5.29 could be significantly varied by proper adjustment of the left side member. The variability could be achieved if one imagines that as the concentration wave moves smoothly down the column at a given temperature, the solute molecules undergo a series of stop-and-go behavior. In actuality, nonequilibrium exists in most physical systems, since the concentration of the components continually upsets the equilibrium. As a result of this constant movement of concentration waves, full equilibrium is prevented. Therefore it is clear that the amount of product withdrawal determines how slow or fast the movement of a given solute is. If the product withdrawn at a given temperature is small, the solute wave will move slower and conditions of near equilibrium are obtained and therefore high value of $M_i(T)$ (which invariably affects the value of M_i). But, if the product

withdrawn at the same temperature is large, the solute wave will move faster and the conditions far removed from equilibrium are obtained and therefore low value of $M_i(T)$. This characteristic behavior is more pronounced at low temperatures. If there was to be no flow, full equilibrium could be established. Instead of true equilibrium, a steady state condition is obtained where the solutes continuously shift back and forth between the solid and liquid phases at a given temperature.

As would be expected, if a uniform temperature distribution is assumed in the column before the products are withdrawn, the contribution to the nonequilibrium situation by the size of the product withdrawn might be linear. But, if the column is not allowed to attain a uniform temperature distribution before product withdrawal is started, the contribution to nonequilibrium will be nonlinear. The non uniform temperature distribution in the column is more pronounced in the cyclic adsorption process where the product withdrawal is started the moment a new temperature is imposed on the column.

Following Eq. 5.19, for component A to appear in the top product, it means that

$$L_A^I(T_1) - L_A^I(T_2) > 0 \text{ or } L_A^{II}(T_2) - L_A^{II}(T_1) < 0$$

Substituting the penetration distance expressions (Eqs. 5.10 through 5.13) into Eqs. 5.19 and 5.20, it is found that

$$\frac{P_F}{P_{Bott}} > \frac{\Delta t_2}{\Delta t_1} \Delta M_i$$

or

$$P_{\text{Bott}} > C\Delta M_i^{-1} \quad (5.30)$$

where

$$C = \frac{\Delta t_1}{\Delta t_2} P_F \text{ and } P_F = P_{\text{Top}} + P_{\text{Bott}}$$

For symmetrical para pumping operations with constant total feed P_F , C is constant. One can see from Eq. 5.30 that when $P_{\text{Bott}} < C\Delta M_i^{-1}$, both components A and B would appear in the bottom product streams. Therefore for a mixture containing solutes A and B, each with its own ΔM , it follows that

$$C\Delta M_B^{-1} > P_{\text{Bott}} > C\Delta M_A^{-1} \quad (5.31)$$

By proper adjustment of P_{Bott} in Eq. 5.31, a true solute split will be obtained which is analogous to that obtained by a multicomponent distillation column.

The requirement necessary for only component A to appear in the top product corresponds to the Region 1 mode of operation (Chen et al. [1974]) and that it is necessary for both components A and B to appear in the bottom product corresponding to the Region 2 mode of operation. Normal multicomponent mixtures exhibit exothermic heats of adsorption. Therefore equilibrium isotherms $M_i(T)$ and $m_i(T)$ have positive slopes. Some of these components will be in Region 1 and some in Region 2, depending on the values of their ΔM_i and on the manner in which the principal operating parameters P_{Bott} and P_{Top} are selected by the operator. However, mixtures that exhibit endothermic heat of adsorption could be in Region 3 mode of operation (i.e., $L^I_i(T_1)$ and $L^I_i(T_2) > H_{\text{CO}1}$).

Upon rearrangement and integration, the concentration profile can be obtained from Eq. 5.7 viz:

$$\frac{dy_i}{y_i} = - \frac{dm_i}{1 + m_i}$$

or

$$\frac{dy_i}{y_i} = - \frac{(1 - \epsilon)dM_i(T)}{[\epsilon + (1 - \epsilon)M_i(T)]} \quad (5.32)$$

Integrating Eq. 5.32 without definite limits (Pigford et al. [1969]), one gets

$$y_i(z,t)[\epsilon + (1 - \epsilon)M_i(T)] = \text{constant}$$

or

(5.33)

$$y_i(z,t)[1 + m_i(T)] = \text{constant}$$

Equation 5.33 means that the concentration $y_i(z,t)$ will undergo a change in value proportional to ΔM_i at defined by equation 5.25; when the characteristic, pass through a cold region to a hot one, the value of ΔM_i will be large and when the characteristics pass through a hot region to a cold one, the value of ΔM_i will be small. The magnitude of ΔM_i depends on the adsorbent type, the solutes, the solvents, the flow rates, amount of products (P_{Top} and P_{Bottom}) withdrawn, and principally on the temperature.

External Equations

To determine the concentration of components A and B, make a material balance on all streams going in and out of the columns (see Figure 5.4).

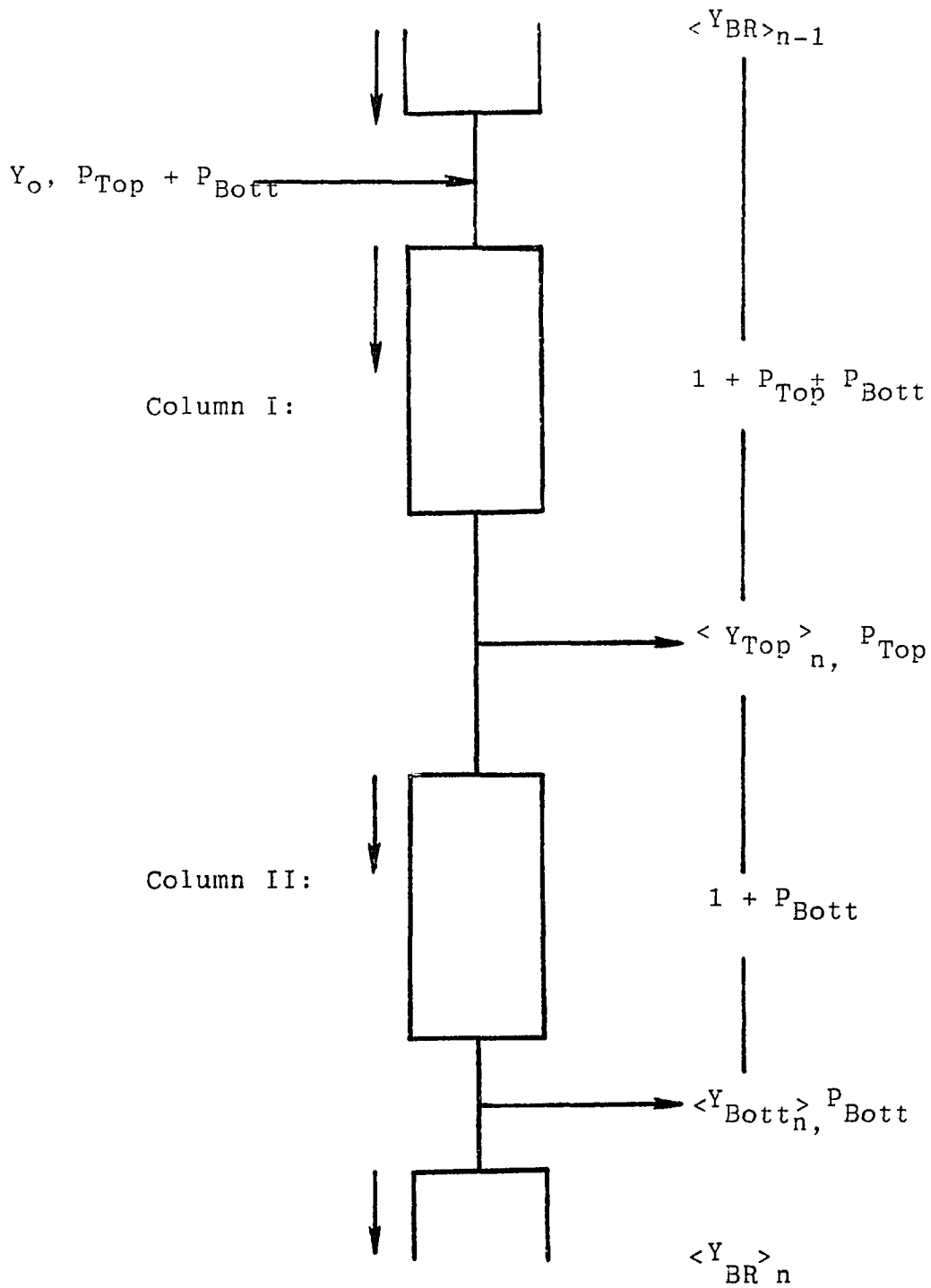


FIGURE 5.2 MATERIAL BALANCE DIAGRAM FOR COLUMNS I & II

Material balance for columns I and II is as follows:

$$\text{I: } (P_{\text{Top}} + P_{\text{Bott}})y_0 + \langle y_{\text{BR}} \rangle_{n-1} = (1 + P_{\text{Top}} + P_{\text{Bott}})\langle y_{\text{Top}} \rangle_n \quad (5.34)$$

$$\text{II: } (1 + P_{\text{Top}})\langle y_{\text{Top}} \rangle_n = \langle y_{\text{B}} \rangle_n(1 + P_{\text{Bott}}) + \langle y_{\text{BR}} \rangle_n \quad (5.35)$$

From Eqs. 5.34 and 5.35,

$$\langle y_{\text{Top}} \rangle_n = \frac{1}{1 + P_{\text{F}}} [(P_{\text{Top}} + P_{\text{Bott}})y_0 + \langle y_{\text{Bott}} \rangle_{n-1}] \quad (5.36)$$

and

$$\langle y_{\text{Bott}} \rangle_n = \langle y_{\text{Top}} \rangle_n - \frac{\langle y_{\text{BR}} \rangle_n}{1 + P_{\text{Bott}}} \quad (5.37)$$

Equation 5.33 implies that for a given temperature and half cycle duration time that

$$y(1 + m_i(T)) = \text{constant}$$

Therefore for the first half cycle duration time, Δt_1 ,

$$y_i \Delta t_1 (1 + m_i(T_{k,j-1})) = \text{constant} \quad (5.38)$$

and for the second half cycle duration time, Δt_2 ,

$$y_i \Delta t_2 (1 + m_i(T_{k,j})) = \text{constant} \quad (5.39)$$

After the temperature change from $T_{k,j-1}$ to $T_{k,j}$, the change in concentration is

$$\frac{y_i \Delta t_2}{y_i \Delta t_1} = \frac{1 + m_i(T_{k,j-1})}{1 + m_i(T_{k,j})} = \Delta M_i \quad (5.40)$$

From Eq. 5.30, and for symmetrical half cycle time (i.e., $\Delta t_1 = \Delta t_2$, and $C = P_{\text{F}}$), at the lower limit, $P_{\text{B}} = P_{\text{F}} \Delta M_i^{-1}$, then

$$P_{\text{Bott}} = P_{\text{F}} \left[\frac{1 + m_i(T_{k,j})}{1 + m_i(T_{k,j-1})} \right] = P_{\text{F}} \Delta M_i^{-1} \quad (5.41)$$

Substitute Eq. 5.41 into Eqs. 5.36 and 5.37 to get

$$\langle y_{\text{Top}} \rangle_n = \frac{y_0}{1 + P_F} \left[(P_T + P_F \Delta M_i^{-1}) + \frac{\langle y_{\text{Bott}} \rangle_{n-1}}{y_0} \right] \quad (5.42)$$

and

$$\langle y_B \rangle_n = \frac{y_0}{1 + P_F} \left[(P_T + P_F \Delta M_i^{-1}) + \frac{\langle y_{\text{Bott}} \rangle_{n-1}}{y_0} \right] - \frac{\Delta M_i \langle y_{\text{BR}} \rangle_n}{P_F + \Delta M_i} \quad (5.43)$$

where

$$\langle y_{\text{BR}} \rangle_n = \langle y_{\text{BR}} \rangle_{n-1} [V_B + Qt]$$

CYCLIC ADSORPTION PROCESS--ONE COLUMN

The cyclic adsorption process developed for the separation of liquid mixtures is shown in Figure 5.5. The preliminary work done consists of a one column process similar to Wakat (1978) and his co-workers, and Barker III and Pigford (1971). The feed at a constant concentration y_0 is introduced into the column at a flowrate Q volume units per unit time. The duration time of each cycle is t_n time units, n equals the number of temperature steps, therefore the displacement volume for a given cycle is Qt_n . The temperature of the bed which is cyclically altered consists of a series of temperature step inputs. At the end of the upper temperature input, the temperature input is down stepped to the lowest temperature and the series of temperature step inputs is again started. For the one column process, samples are continuously collected and analyzed for the effluent concentration. Cyclic changes are obtained as a result of the cyclic temperature inputs. The series of temperature imposed on the column is determined by the number of solutes in the fluid

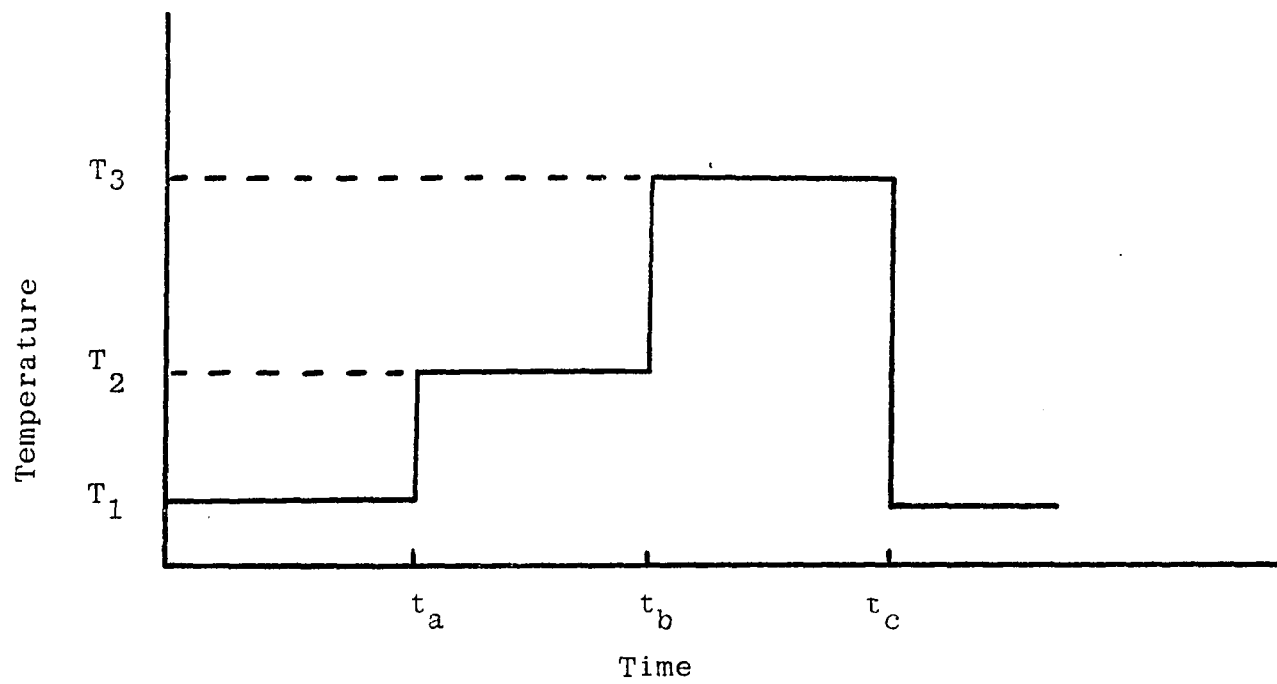


FIGURE 5.3 STEPWISE TEMPERATURE PROFILE APPLIED TO COLUMN

mixture. The lowest temperature is chosen so that all solutes are adsorbed. The highest temperature is picked so that all solutes are completely desorbed. By such careful selection of the lowest and highest temperature levels, all the solutes will be concentrated between the lowest and highest temperatures. The intermediate temperatures will have to be chosen so that the solutes will be selectively fractionated depending on the penetration distances $L_i(T)$ at the given temperature. The penetration distance of individual solutes in the column depends on the equilibrium distribution of each solute between stationary and mobile phases. Therefore successful fractionation is determined by those experimental variables that affect this distribution, the composition of the solutes in the fluid mixtures, the composition of the solutes in the stationary phase, volumetric flowrate, and the separation temperature.

In the local equilibrium theory (Pigford [1969]) used in the analysis of the separation phenomenon, the effect of the concentration of the solutes is assumed to be negligible. The principal variables that affect the distribution of the solutes and therefore the penetration distance, is the temperature input and the fluid volumetric flow rate. As a given solute concentration wave front penetrates through the column at a given temperature, the distances moved by the molecules of each solute are not identical. The differences in molecular penetration distances for molecules of each solute do not arise from differences in equilibrium distribution, rather, it is caused by physical or rate processes.

The important physical processes which affect the molecular penetration distances could be classified into five categories:

- (a) Eddy diffusion (or multiple flowpaths): This phenomenon arises from the fact that the fluid mixtures flow through microscopic pathways through the packed bed. The molecules will move through wide pathways faster, and slower through narrow pathways. So the magnitude of eddy diffusion depends on the particle size and how well the column is packed.
- (b) Liquid phase mass transfer: The mass transfer of the liquid depends on differing flow rates of different parts of a single microscopic pathway. Solute molecules adjacent to adsorbent particles move slower than those in the center of a flowstream.
- (c) Intraparticle mass transfer: This is more pronounced if the adsorbent particle consists of porous particles. Solute molecules move in and out of these pores by diffusion. Certain solute molecules will diffuse in and out of the pores faster than others. The molecules that diffuse faster will penetrate down the column more than those that diffuse slower.
- (d) Solid-phase mass transfer: The solute molecules that are in the pores diffuse further into the solid part of the adsorbent. The longer the molecules take in returning to the fluid phase, the shorter the distance penetrated by such molecules down the column.

- (e) Longitudinal diffusion (or axial diffusion): This is the random movement of solute molecules in all directions. The effect of longitudinal diffusion could be very significant at low flow rates and small adsorbent particles.

The equilibrium distributions are also a directional function of the excess free energies of adsorption (ΔG) of the fluid mixtures, which are a direct measure of the net forces holding the solutes to the adsorbent. Although the chemical nature of the solutes may differ, two solutes in a given liquid-solid system may have the same partition coefficient, $k = KV_S/V_m$ (K = equilibrium distribution coefficient, V_S = volume of solute in solid phase, and V_m = volume of solute in mobile phase), in which case, one may be held predominantly by nonpolar forces and the other by polar forces. The sequence of temperature chosen must be such as to be able to progressively decrease the dispersive forces and therefore the equilibrium distribution coefficient.

The penetration distance equation as defined in Eq. 5.9 also applies to the cyclic adsorption process. Figure 5.4 shows the steady state characteristic solution for the cyclic adsorption process. From Eq. 5.9, it is shown that if the average bulk velocity of the fluid within the column is v cm/sec, the concentration wave velocity of solute i is u_{con} , cm/sec, then the solute wave will penetrate down the column a distance $L_i(T)$. To be able to collect samples concentrated in a desired component, it becomes a matter of necessity to be able to predict the time

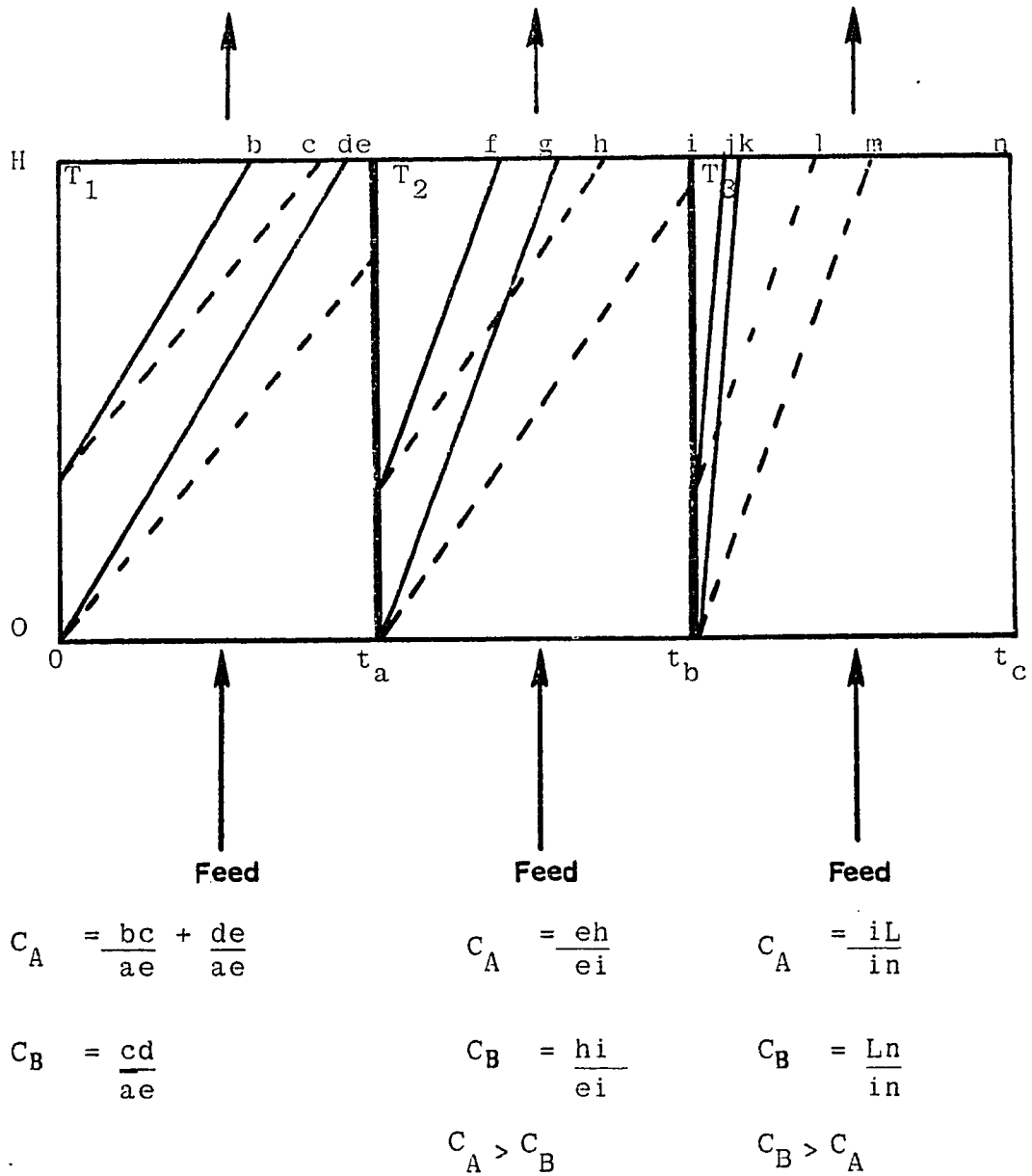


FIGURE 5.4 **STEADY STATE CHARACTERISTIC SOLUTION FOR ONE COLUMN ADSORPTION PROCESS**

required for the solute wave to exit the length of the column. Upon rearrangement of Eq. 5.9,

$$\frac{L_i(T)}{\Delta t} = \frac{v}{1 + \frac{(1 - \epsilon)}{\epsilon} M_i(T)} = u_{con} \quad (5.9a)$$

Now, define $\bar{\theta}_i$ = average time required for the center of the band to exit the height of the column, H_{col} , after a temperature change. Since time equals distance divided by velocity,

$$\bar{\theta}_i = \frac{H_{col} \Delta t}{L_i(T)} \quad (5.44)$$

To express $\bar{\theta}_i$ as a function of the fundamental column parameters H_{col} , $M_i(T)$ and ϵ , we have

$$\bar{\theta}_i = \frac{H_{col} [\epsilon + (1 - \epsilon) M_i(T)]}{\epsilon v} \quad (5.45)$$

To collect concentrated samples over a given period of time, Eq. 5.45 can be rewritten,

$$\bar{\theta}_i \pm \sigma = \frac{H_{col} [\epsilon + (1 - \epsilon) M_i(T)]}{\epsilon v} \quad (5.46)$$

Where σ is the time deviation from $\bar{\theta}_i$, and $\bar{\theta}_i - \sigma$ is the average time when product withdrawal is started, and $\bar{\theta}_i + \sigma$ is the average time at which product withdrawal is ended.

Internal Equations

From Eq. 5.9, it becomes apparent that to separate a given solute A from the solvent, two temperature levels T_1 and T_2 are required ($T_1 < T_2$) with corresponding solute concentration wave penetration distance L_1 and L_2 , therefore we must have,

$$L_1 < H_{CO1} < L_2 \quad (5.47)$$

For two solutes, three temperature levels are required, $T_1 < T_2 < T_3$, and the following inequality criteria must be satisfied:

$$\begin{aligned} (L_A)_1 &< H_{CO1} < (L_A)_2 \\ (L_B)_2 &< H_{CO1} < (L_B)_3 \end{aligned} \quad (5.48)$$

and

$$(L_B)_2 < H_{CO1} < (L_A)_2$$

Equation 5.48 states that for solute A to be fractionated from solute B, the penetration distance of solute A at T_2 must be greater than the height of the column and the penetration distance of solute B at T_2 must be less than the height of the column. The principal operating parameters must be chosen so that solute A could exit the column at temperature level T_2 while solute B does not, and solute B should exit the column at temperature level T_3 . Temperature level T_1 must be low enough so that the exiting fluid will have a low concentration in both solutes. If the time duration at which T_1 is imposed is long enough, the exiting solute concentration would rise and finally correspond to the feed concentration. Therefore it is extremely critical to choose cycle duration time to prevent this occurrence. The reasoning for the development of the inequality criteria for two solutes could be extended to a number of solutes. For i -solute systems, the following criteria must be satisfied to be able to fractionate them into a variety of fractions.

$$(L_1)_1 < H_{CO1} < (L_1)_2$$

$$(L_2)_2 < H_{CO1} < (L_2)_3$$

$$\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{array}$$

$$(L_i)_N < H_{CO1} < (L_i)_{N+1}$$

and

$$(L_2)_2 < H_{CO1} < (L_1)_2 \tag{5.49}$$

$$(L_3)_3 < H_{CO1} < (L_2)_3$$

$$\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \end{array}$$

$$(L_i)_N < H_{CO1} < (L_{i-1})_N$$

where

i = number of solutes

N = number of temperature levels

Now that the necessary conditions for the fractionation have been established, there are certain practical limitations that must be taken into account. These limitations are as follows: the solvent should be generally inexpensive; the solvent should be non polar to avoid competition between solvent and solute for adsorption site; a mixture of solvents should be avoided to prevent demixing normally found in liquid-solid chromatography; and the solvent should have low viscosity to ensure rapid mass transfer and thus adequate column efficiency. The solvent should be significantly less volatile than any solute thereby rendering recovery of solute via distillation practicable without the necessity to employ substantial fractional distillation or to expend energy evaporating solvents.

CYCLIC ADSORPTION PROCESS--MULTICOLUMN

The simulated one column cyclic adsorption process which is operated semi-continuously, (fluid mixture fed into the column continuously, but product is not withdrawn continuously) is extended to staged sequence cyclic adsorption. With the staged sequence cyclic adsorption, the process is operated continuously in that the fluid mixtures are fed into the columns and product withdrawn continuously. This process is, in essence, a simulated moving bed. The true continuous nature of the process eliminates the mixed reservoirs normally used in parametric pumping, since reservoir mixing tends to reduce separation (Rice and Foo [1981]). Separation of a mixture of i solutes by the direct-mode of operation requires a set-up with $n+1$ columns and N driving forces. The feed and product ports are fixed in the staged sequence process, but different components can be directed to exit from specified ports by synchronizing the feed and product positions with the appropriate intensive variable (in this work, a series of temperature step inputs). For a complete analysis of the internal equations, Eqs. 5.47 through 5.49 and Table 5.2 give all the details of the events occurring in the columns.

External Equations

The analysis of the phenomenon of fractionation is incomplete without the external equations. Figure 5.7 shows the schematic of the staged sequence adsorption process. We can write the mass balance at Δt_1 time cycle.

TABLE 5.2

CHARACTERISTICS OF A STAGED SEQUENCE ADSORPTION PROCESS

Stage no	$\left\{ \begin{array}{l} \frac{L_i(T)}{v\Delta t_1} \\ \frac{L_i(T)}{v\Delta t_2} \\ \frac{L_i(T)}{v\Delta t_3} \end{array} \right.$	$\frac{R_n P_T + P_F}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_1)}$	$\frac{P_T}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_2)}$	$\frac{R_T P_T}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_3)}$	Penetration Distance Inequalities for Solutes A and B, $M_B(T) > M_A(T)$
Column I		$\frac{R_n P_T + P_F}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_1)}$	$\frac{P_T}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_2)}$	$\frac{R_T P_T}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_3)}$	$L_A(T_2) > H_{col}$ $L_B(T_2) < H_{col}$ $L_A(T_3) > H_{col}$ $L_B(T_3) < H_{col}$
Column II		$\frac{R_n P_T + P_F}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_2)}$	$\frac{R_B P_B}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_3)}$	$\frac{R_B P_B + P_B}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_1)}$	$L_A(T_2) > H_{col}$ $L_B(T_2) < H_{col}$ $L_B(T_3) > H_{col}$ $L_A(T_1), L_B(T_1) < H_{col}$
Column III		$\frac{R_I P_I}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_3)}$	$\frac{R_I P_I + P_F}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_1)}$	$\frac{P_I}{1 + (\frac{1-\epsilon}{\epsilon}) M_i(T_2)}$	$L_A(T_2) > H_{col}$ $L_B(T_2) < H_{col}$ $L_B(T_3) > H_{col}$ $L_A(T_1), L_B(T_1) < H_{col}$

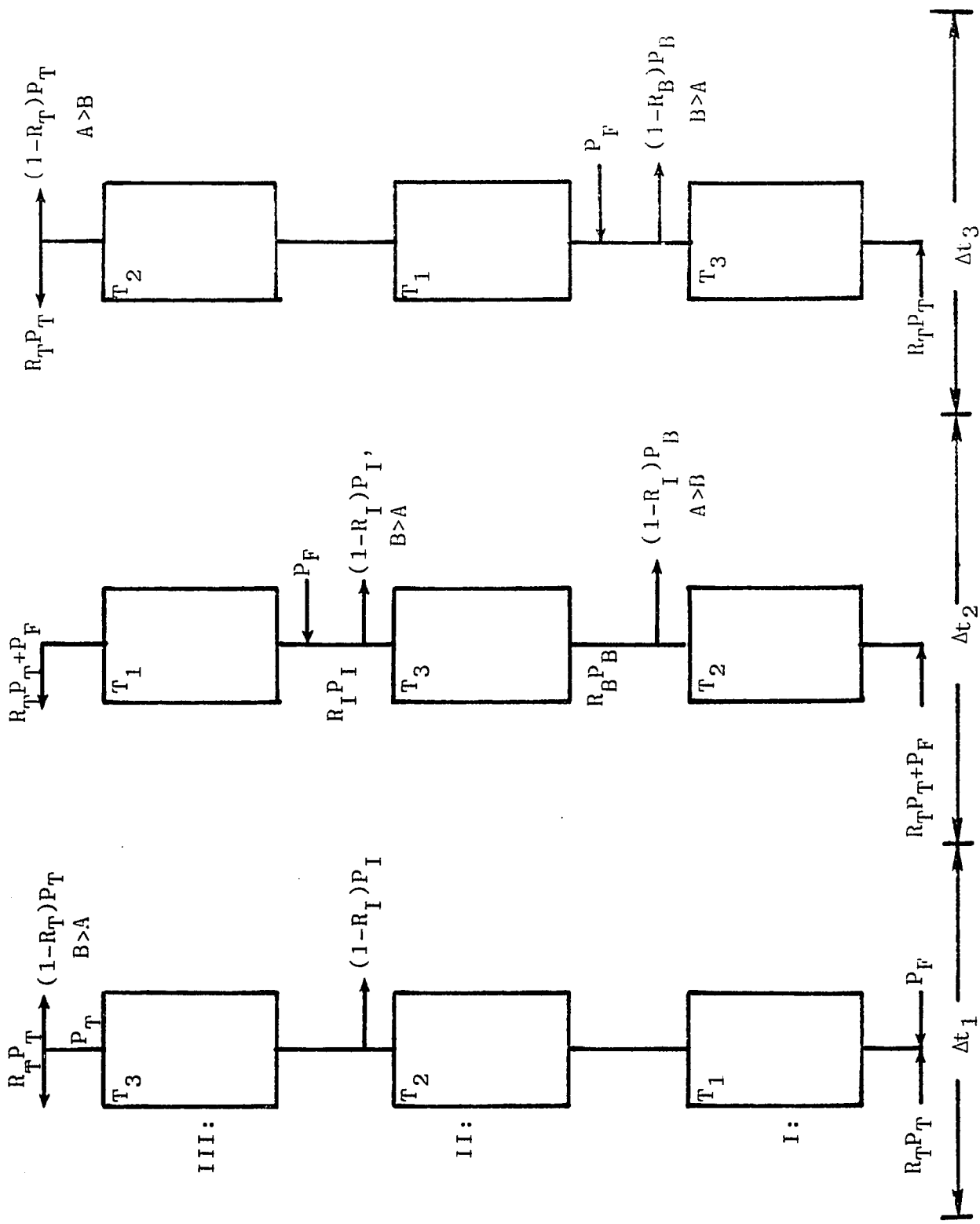


FIGURE 5.5 MATERIAL BALANCE DIAGRAM FOR STAGED SEQUENCE CYCLE PROCESS

$$\text{Column 1: } P_F + R_T P_T = P_B \quad (5.50)$$

$$\text{Column 2: } P_B = F_I \quad (5.51)$$

$$\text{Column 3: } R_I P_I = P_T \quad (5.52)$$

Combine Eqs. 5.50 and 5.51

$$P_F + R_T P_T = P_I \quad (5.53)$$

Combine Eqs. 5.52 and 5.53

$$P_F + R_T R_I P_I = P_I$$

or

$$P_I = \frac{P_F}{1 - R_T R_I} \quad (5.54)$$

Combine Eqs. 5.52 and 5.54 to get

$$P_T = \frac{P_F R_I}{1 - R_T R_I} \quad (5.55)$$

The solute concentrations are obtained by making a solute material balance on the entire system. A solute balance for nth cycle, considering columns 1 and 2, we obtain

$$\begin{aligned} \langle y_I \rangle_n P_I &= \langle y_B \rangle_n P_B \\ &= \langle y_B \rangle_n [P_F + R_T P_T] \\ \langle y_I \rangle_n &= \langle y_B \rangle_{n-1} \left[\frac{P_F + R_T P_T}{P_I} \right] \end{aligned} \quad (5.56)$$

Considering the three columns,

$$\langle y_T \rangle_n P_T = P_F y_F + \langle y_T \rangle_{n-1} R_T P_T - \langle y_I \rangle_n (1 - R_I) P_I \quad (5.57)$$

Substitute Eqs. 5.55 and 5.56 into Eq. 5.57 to obtain

$$\langle y_T \rangle_n = y_F \left(\frac{1}{R_I} - R_T \right) + \langle y_T \rangle_{n-1} R_T + \langle y_B \rangle_{n-1} \left(1 - \frac{1}{R_I} \right) \quad (5.58)$$

Solute concentration transients can be calculated for $\langle y_I \rangle_n$ and $\langle y_T \rangle_n$ for cycle time Δt_1 . Similar solute concentration equations can be derived for subsequent cycle times.

CHAPTER 6

PROCESS DESCRIPTION

PARAMETRIC PUMPING

The configuration of the parametric pump considered is shown in Figure 6.1. The material to be separated is pumped through the column system between the reservoirs during upflow and downflow at a volumetric flow rate Q . Each half cycle time is t , and the columns operate with a displacement volume Qt . The reservoirs at the outer ends of the columns have dead volumes $V_B=V$, and the inner ends of the columns are attached to each other with minimal dead volume. This back-to-back arrangement in an open parametric pumping would minimize reservoir mixing (Thompson and Bowen, 1972). The two columns are operated at 180° out of phase thermally, and arranged in such a fashion that a feed is alternately delivered to the outer ends of the columns at T_1 ($T_1 < T_2$).

The flow rates within the columns are $(1+P_T+P_B)Q$ at T_1 , and $(1+P_B)Q$ at T_2 for the upper and lower columns respectively during downflow. During upflow, the respective column flow rates for the upper and lower columns are reversed, i.e. $(1+P_B)Q$ at T_2 , and $(1+P_T+P_B)Q$ at T_1 . The feed which is only introduced to the outer end of a column at T_1 has a flow rate $(P_T+P_B)Q$. The top and bottom product flow rates are P_TQ and P_BQ respectively. Material balance around the point of entry of the feed and point of upper column product withdrawal during both downflow and upflow show that the flow rate must be $(1+P_T+P_B)Q$, while the flow rate at the

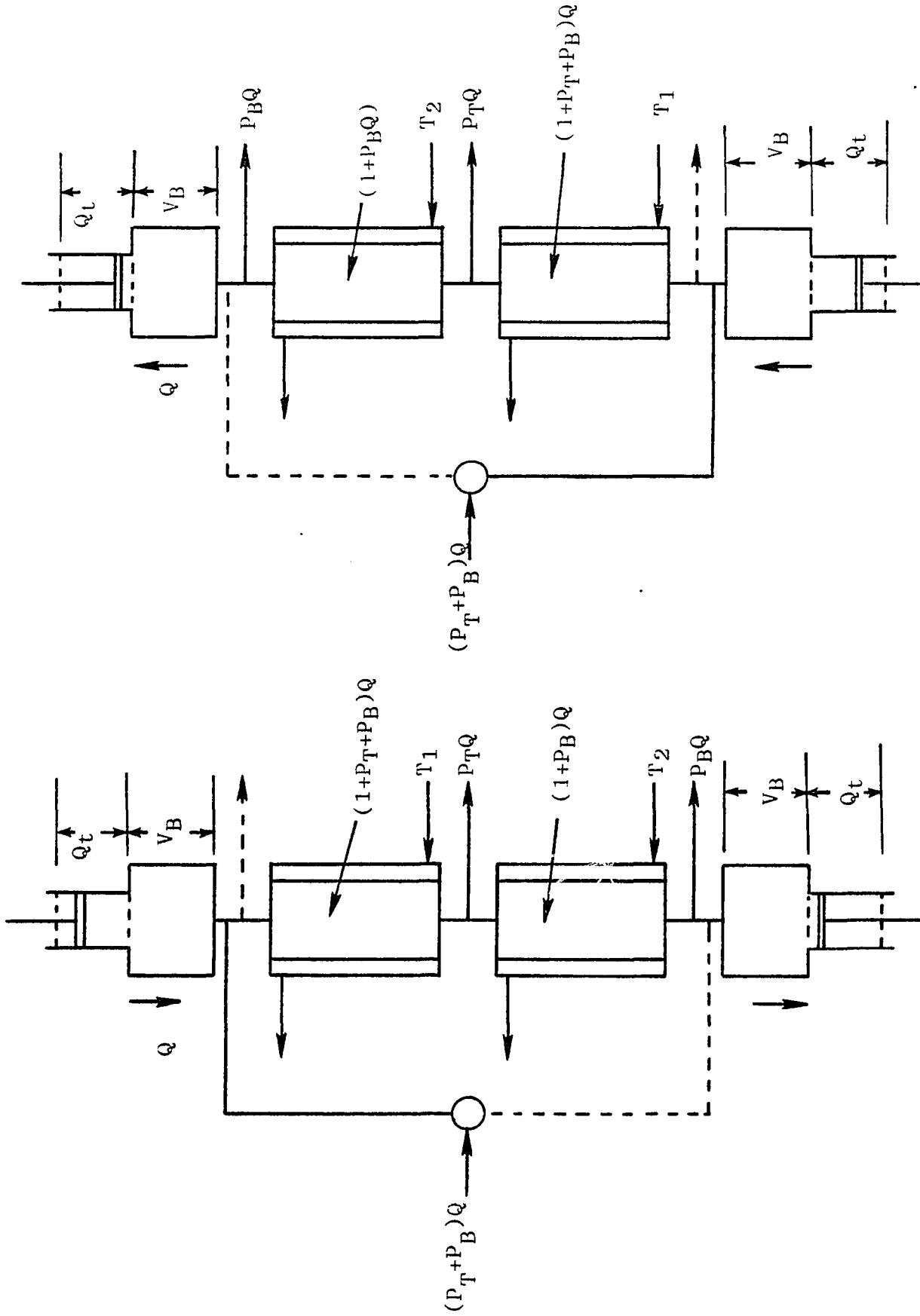


FIGURE 6.1 INTERNAL FLOW RATES IN A TWO COLUMN PARAMETRIC PUMP WITH ALTERNATING TOP FEED

point of bottom product withdrawal must be $(1+P_B)Q$.

The two columns are assumed to be filled with the adsorbent particles; the column voids and both reservoirs are filled with fluid mixtures consisting of a three component mixture, two components of which are assumed to distribute between the liquid and solid phases. The bottom product stream (taken from outer ends of columns) during both downflow and upflow comes only through the columns and not from the reservoirs or directly from the feed stream. The top product stream (inner ends of the columns) during both downflow and upflow also comes through the columns. Our interest will be focused primarily on the effluents leaving the inner ends of the columns where minimum mixing is assumed to occur. Component A is to be concentrated at the inner ends of the columns in both downflow and upflow. It is assumed that the concentration of each band of component A at the inner ends of the columns is not mixed (i.e. plug flow), except when the top product is taken. Component B is to be concentrated at the outer ends of the column in both downflow and upflow. The concentrations of the bands taken as bottom products are assumed to be perfectly mixed after the bottom product is withdrawn.

STAGED SEQUENCE CYCLIC PROCESS

In principle, the staged sequence cyclic process is a simulated moving bed. The advantages claimed for this process is the combination of the inherent selectivity and separation capabilities of a chromatographic column; elimination of a

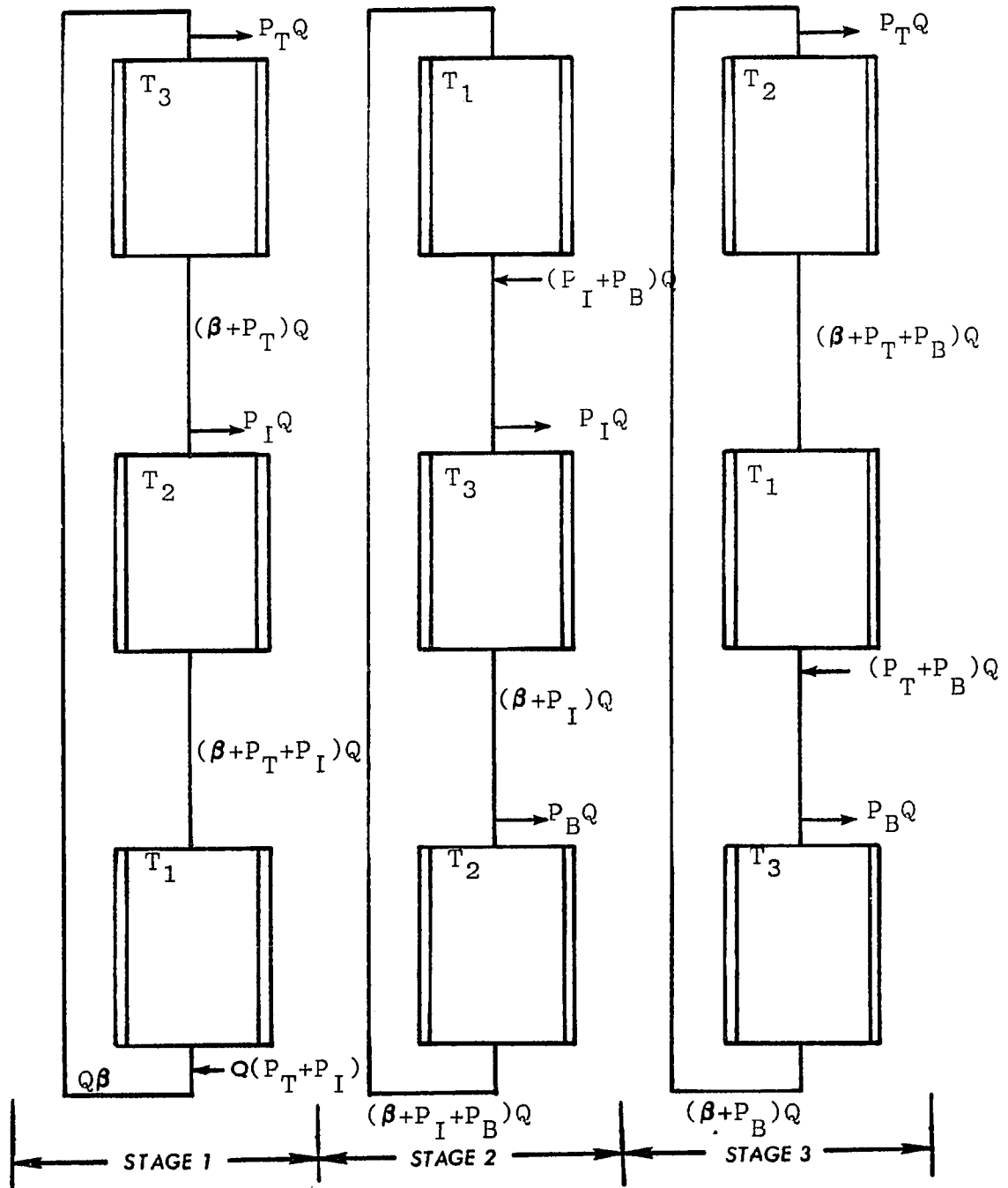


FIGURE 6.2 COLUMN ARRANGEMENT FOR STAGED SEQUENCE CYCLIC PROCESS

desorbent normally employed in a conventional or simulated moving bed operation to displace feed components in the column, application of temperature cycling as the only force used to attain adsorption and selective desorption, a continuous fractionation of multicomponent solutions into a variety of fractions, and the elimination of reservoir mixing normally found in parametric pumping.

The schematic for the staged sequence cyclic process is shown in Figure 6.2. The temperature cycling consists of a series of temperature steps sequentially imposed on the columns. The process consists of three distinct stages. Each stage consists of $n+1$ simultaneous operations. To fractionate n components, $n+1$ columns are arranged in a series and $n+1$ temperature step inputs are required. The fractionation process is achieved by operating the columns in such a fashion that each column experiences a sequential temperature input. The temperatures must be chosen so that, at the lowest temperature, the penetration distance, $L_i(T_1)$, of all components in the solution is less than the height (H_{CO1}) of the column. For this study, columns of equal heights are used; however, columns of unequal height could also be used. If we consider a mixture containing i solutes, each solute with its own $L_i(T_N)$, the temperatures must be chosen so that

$$\begin{array}{l}
L_1(T_1) < H_{\text{col}} < L_1(T_2) \\
L_2(T_2) < H_{\text{col}} < L_2(T_3) \\
\vdots \\
\vdots \\
\vdots \\
L_i(T_N) < H_{\text{col}} < L_i(T_{N+1})
\end{array} \quad (6.1)$$

and

$$\begin{array}{l}
L_2(T_2) < H_{\text{col}} < L_1(T_2) \\
L_3(T_3) < H_{\text{col}} < L_2(T_3) \\
\vdots \\
\vdots \\
\vdots \\
L_i(T_N) < H_{\text{col}} < L_{i-1}(T_N)
\end{array} \quad (6.2)$$

Following the supposition that the fluid mixtures to be separated contain species A and B with penetration distances $L_A(T)$ and $L_B(T)$ where as $L_A(T) > L_B(T)$ and specifically,

$$\begin{array}{l}
L_A(T_1) < H_{\text{col}} < L_A(T_2) \\
L_B(T_2) < H_{\text{col}} < L_B(T_3)
\end{array} \quad (6.3)$$

and

$$L_B(T_2) < H_{\text{col}} < L_A(T_2) \quad (6.4)$$

then, at T_1 , the solution is fed to column 1 and components A and B are simultaneously released from columns 2 and 3 respectively; these columns are respectively at T_2 and T_3 . As a result, the fluid exiting from column 1 will have low solute concentrations; the effluent from column 2 has high concentration in solute A and low concentration in B; and fluid with high concentration of solute B and low concentration of solute A is withdrawn from column 3. If the process is properly timed, the band of high concentration of both solutes can be withdrawn as samples, while

the portion low in solute concentration is recycled. The duration of each stage is crucial, since with long duration times, the exiting solute concentration would approach the feed concentration. A chronological description of the temperature cycling and internal equations as found in the staged sequence cyclic process is described below.

The columns are initialized with the feed solution at T_3 , and the operational steps of the staged sequence cyclic process is as follows:

Stage 1: Operating temperature regiments are imposed on the columns in the following sequence: Column 1($T_3 \rightarrow T_1$), Column 2($T_1 \rightarrow T_2$), and Column 3 ($T_2 \rightarrow T_3$)(where the arrow means change). The flow rate in column 1 is $(\beta + P_I + P_T)Q$, β is the amount of fluid recycled from column 3; P_I is the amount of product to be withdrawn from column 2 at T_2 ; P_T the amount of product to be withdrawn from column 3 at T_3 ; and $(P_I + P_T)Q$ is the amount of fresh feed delivered into the system as make up fluid. Since no product is withdrawn from the exit of column 1, the flow rate in column 2 is identical to that in column 1. All the dilute material from column 1 is introduced into column 2. At the exit of column 2, the flow rate of the product withdrawn is $P_I Q$ and the remaining portion, $(\beta + P_T)Q$ is now the feed into column 3. The top product with a flow rate equal to $P_T Q$ is withdrawn from column 3. As can be seen from the ongoing analysis, the flow rate in column 3 is not equal to the flow rate in columns

1 and 2, other arrangements where the flow rates are equal are possible.

Stage 2: For this stage, the column operating temperatures are switched in the following order: Column 1 ($T_1 \rightarrow T_2$), column 2 ($T_2 \rightarrow T_3$) and column 3 ($T_3 \rightarrow T_1$). The flow rate of the material in column 3 which is now the input, and therefore the flow rate of the material in column 1 is $(\beta + P_B + P_I)Q$. The amount of product (rich in component A) to be withdrawn from column 1 is $P_B Q$, while the remaining portion, $(\beta + P_I)Q$, is input to column 2. Products rich in component B at a flow rate of $P_I Q$ is withdrawn at the exit of column 2, and the balance βQ combined with the make up fluid, $(P_I + P_B)Q$ is now the feed and therefore the flow rate of the fluid in column 1.

Stage 3: This is the last stage in the staged sequence cyclic process. The column temperatures are switched as follows: Column 1 ($T_2 \rightarrow T_3$), column 2 ($T_3 \rightarrow T_1$) and column 3 ($T_1 \rightarrow T_2$). The amount of material being delivered into column 1 from the exit of column 3 is $(\beta + P_B)Q$. At the exit of column 1, the bottom product, at a rate of $P_B Q$, is withdrawn and the remaining material, βQ , is combined with $(P_T + P_B)Q$ and fed into column 2. At the exit of column 2, no product is withdrawn--all of the exiting material goes to column 3. Exiting from column 3 is material rich in component A and the top product is withdrawn at a rate of $P_T Q$, while the rest is recycled to column 1. These stages consist of the first cycle, and for subsequent cycles, stages 1 through 3 are repeated.

CHAPTER 7

PROCESS OPERATION

PARAMETRIC PUMPING

The preliminary parapumping work done was with one column with top feed identical to that used by Chen et al. (1972, 1973) and Stokes (1976). The description of the one column experimental set up will not be repeated, but the two column parametric pump employed thereafter with alternating top feed apparatus shown in Figure 7.1 will be offered. The equipment consists of two jacketed glass columns each 1.0 cm in diameter and 90 cm long packed with 30-60 mesh chromatographic-grade silica gel manufactured by Fisher Scientific. The two bottom reservoirs at the outer ends of the columns were two 50 cc glass syringes operated by a dual infusion-withdrawal pump manufactured by the Harvard Apparatus Company. The pump circuit was modified by wiring a micro-switch to automatically reverse the syringes at the completion of each cycle.

The jacketed columns were heated and cooled by pumping water from constant hot and refrigerated baths maintained at constant temperatures of approximately 70°C and 30° respectively. The heating and cooling process was accomplished by direct piping from the baths to the column using a series of solenoid valves to direct the heating or cooling fluids in and out of the columns. The solenoid valves were wired to timers so that the heating and cooling of the columns could be achieved at 180° thermally out of phase.

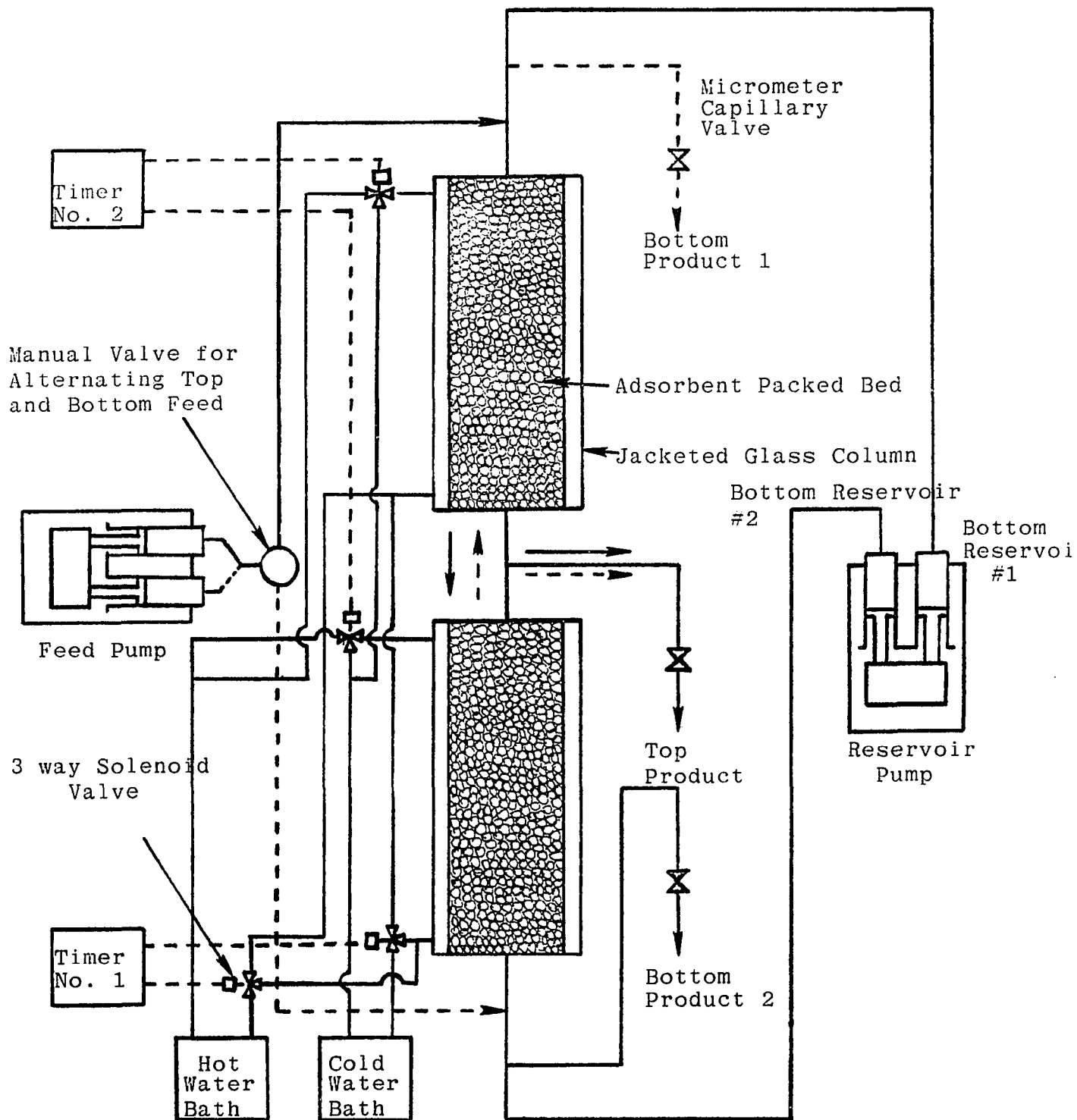


FIGURE 7.1 EXPERIMENTAL APPARATUS FOR ALTERNATING TOP FEED THERMAL PARAMETRIC PUMPING

The feed solution was alternately delivered to the top of the column that is being cooled. A manual valve was used to change the flow direction of the feed solution from two 50 cc syringes mounted in a second infusion-withdrawal pump, and one syringe was used as a back-up for the other. This arrangement eliminated abrupt interruptions of the pumping process for periodic refilling of the feed syringe. By so doing, the possibility of destroying the waves and therefore causing internal mixing of the concentration bands is eliminated. Micrometer capillary valves were used to regulate the flow rates of the top and bottom product streams. Thermal expansion and contraction of the fluid mixture and packing material which occurs due to periodic temperature change causes air to enter the system. The presence of air in the system reduces mass transfer considerably. This problem could be corrected by using the micrometer capillary valves to impose a back pressure on the column to compensate for the expansive and contractive effects caused by temperature changes.

Prior to each run, the column was slurry packed with silica gel in the feed solution and carefully degased. The two reservoirs, feed pumps and all connecting lines were filled with the feed mixture at ambient temperatures. The reservoir delivery rate was set allowing a dead volume of about 10 cc.

To begin each run, the heating and cooling fluid delivery pumps were started and the heating and cooling fluid directed to the desired column. The feed and reservoir pumps are switched

on and the timers activated: The effluent from the bottom reservoir is mixed with the feed and fed into the first column while the pumping direction is downward, and the top and bottom products are simultaneously withdrawn. At the end of the first half cycle, the microswitch wired to the pump automatically reversed the pumping direction of the reservoir syringes, while the timer switched the solenoids to supply cold water to the jacket of column 2 and hot water to column 1. Simultaneously, the feed was directed to the top of column 2 and products withdrawn from the top and bottom. The samples to be analyzed are taken from the top and bottom streams at the end of each cycle, and analyzed by gas chromatography.

STAGED SEQUENCE CYCLIC PROCESS

The experimental part of the staged sequence cyclic process was done with a single column and the data used to simulate a continuous multicolumn staged sequence cyclic operation. The experimental apparatus for the single column process is shown in Figure 7.2. The equipment consists of a jacketed stainless steel column 1.0 cm in diameter and 90 cm long, fitted with appropriate stainless steel swagelok tube fittings equipped with sintered discs. The column was packed with 30-60 mesh chromatographic grade silica gel taken from the same stock as that used for the parametric pumping runs. Before packing, the silica gel was activated in a vacuum oven for 24 hours at 100°C to extract water vapor and related soluble materials that may block the adsorption sites of the adsorbent particles.

3 way Solenoid Valves

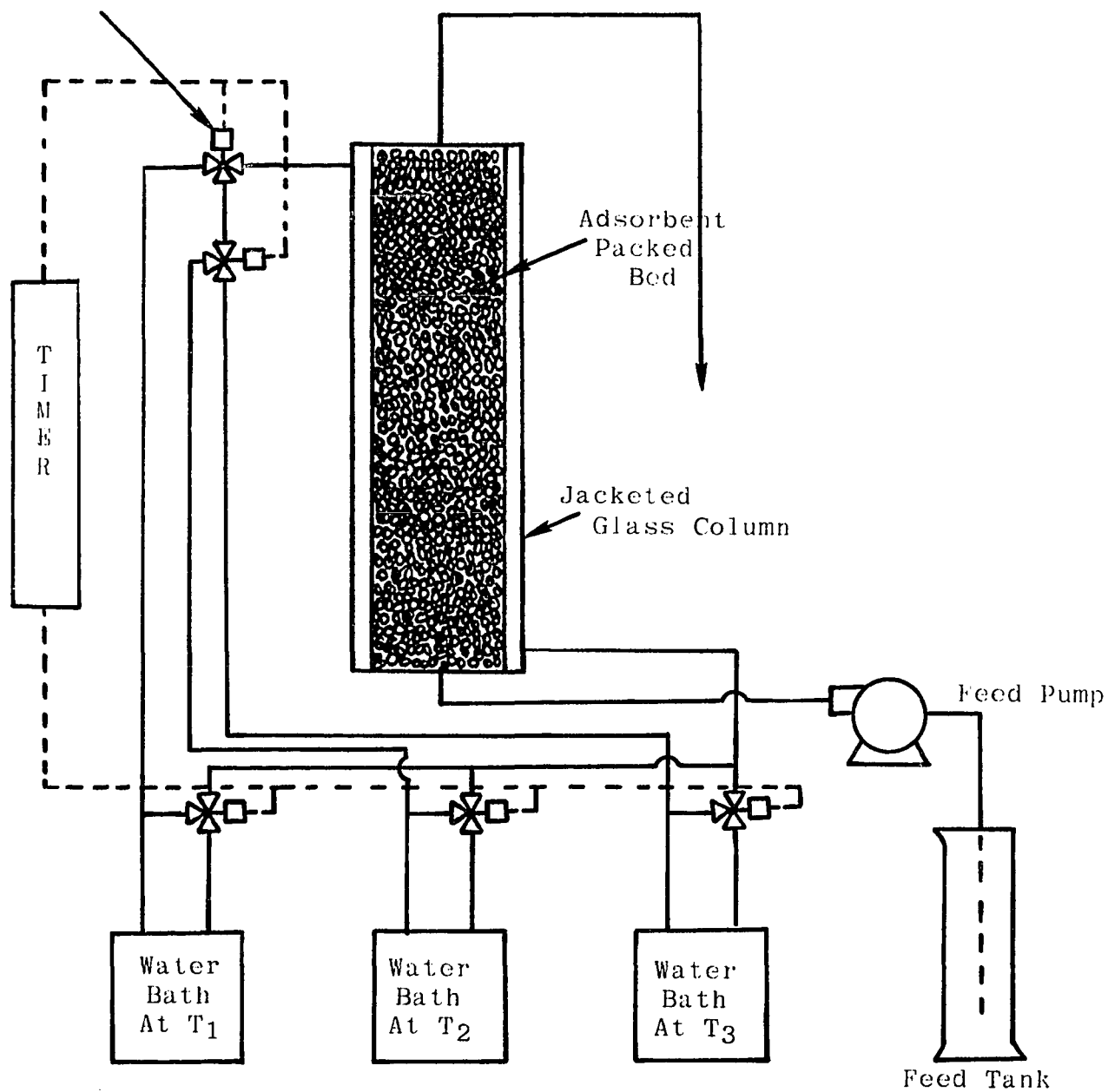


FIGURE 7.2 EXPERIMENTAL APPARATUS FOR ONE COLUMN USED IN SIMULATING STAGED SEQUENCE CYCLIC PROCESS

The jacketed column was heated or cooled by three constant temperature baths maintained at approximately $T_3(=85^{\circ}\text{C})$, $T_2(=60^{\circ}\text{C})$, and $T_1(=30^{\circ}\text{C})$. The baths are piped to the column via a series of solenoid valves connected to programmable timers to heat/cool or recycle the heating/cooling fluid.

The feed solution was delivered by a low pressure Milton Roy Mini pump, with all inlet pressures slightly above atmospheric pressure. Sample fractions were collected at regular and predetermined intervals, and analyzed by gas chromatography.

To start the fractionation process, the column was initialized at $T_3(T_3>T_2>T_1)$. The temperature in the column was then downstepped to T_1 , while the feed solution is fed continuously to the column for a predetermined period of time, and sample fractions continuously taken for analysis. At the end of the sampling period at T_1 , the temperature of the column is changed to T_2 while the feeding and sampling process was continued. And, finally, the column temperature is changed to T_3 . At the completion of the sampling period, one set of temperature cycling is completed. For subsequent sets of temperature cycling, a down step in temperature was made to T_1 and the entire process was repeated.

After establishing the peaking period of the solutes as a result of the temperature cycling, sample products are then withdrawn over a given appropriate interval to collect high product concentrations in component A at T_2 and in component B at T_3 . However, fractionation with this arrangement is a semicontinuous process in that when the column is at T_1 , no

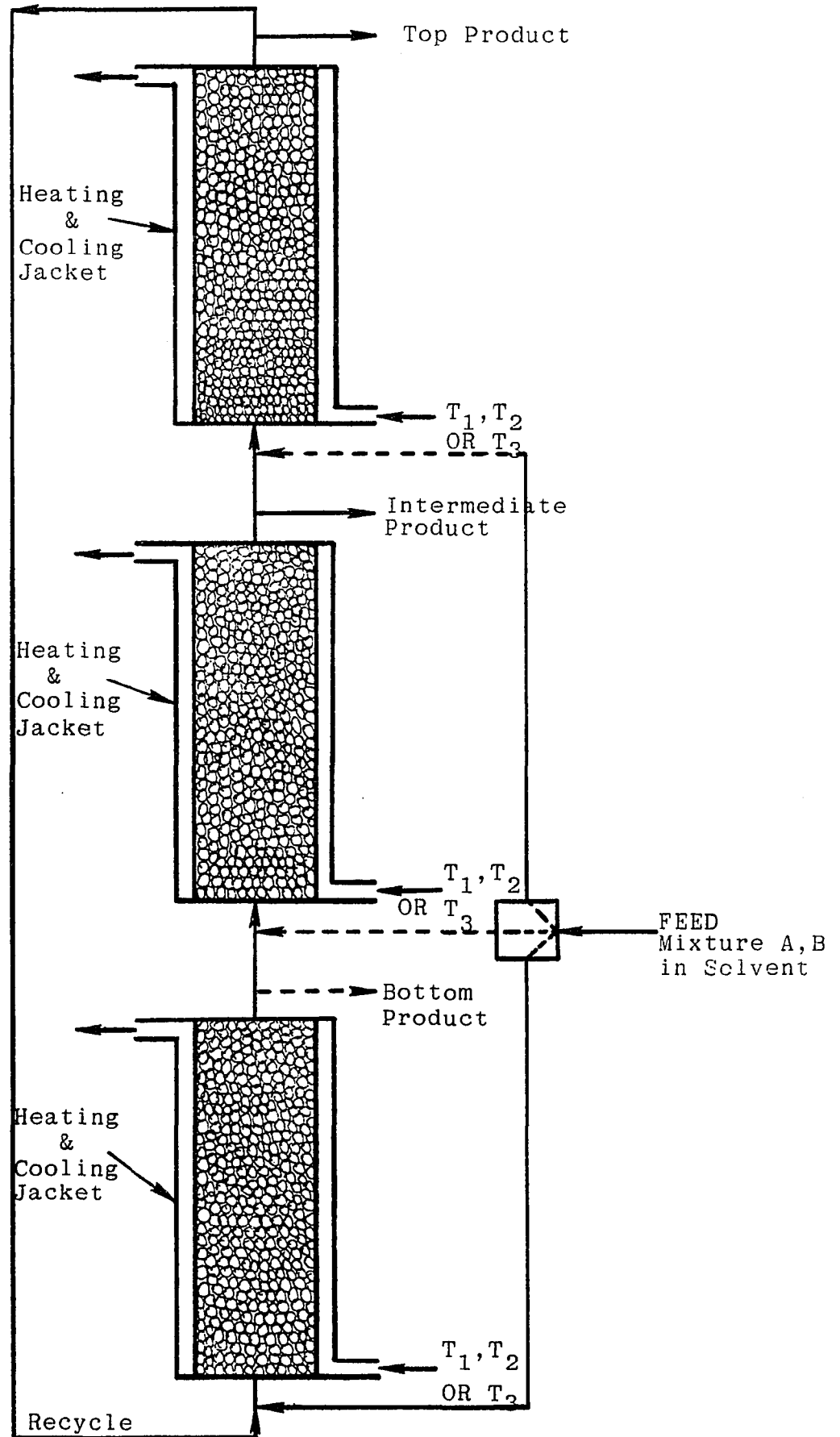


FIGURE 7.3 SCHEMATIC OF STAGED SEQUENCE CYCLIC PROCESS FOR THE CONTINUOUS FRACTIONATION OF SOLUTES A AND B.

sample products were withdrawn. When the column is at T_2 , sample products with concentration high in A was only withdrawn, while at T_3 , product high in component B was withdrawn.

To continuously fractionate the solutes in a true continuous fashion, a schematic diagram shown in Figure 7.3 was used to simulate the one column process. The diagram consists of three stainless steel columns of identical dimensions. This arrangement is advantageous in that high solute product concentrations can be simultaneously obtained.

For the analysis of the sample products, a Hewlett Packard Models 5730A chromatograph and an 3380A integrator were used. Before the analysis of sample products, the flow rate of the carrier gas, in this case helium, was precisely set at 86 cubic centimeters per minute with a bubble flow meter. The oven, thermal conductivity detector, and injection port were maintained at constant temperatures of 250, 200, and 250 degrees Celsius respectively. The detector attenuator was set at a constant value of 1, and the chart speed at 0.5 centimeters per minute. A single column made of 0.635 centimeter o.d. copper tubing of approximately 183 cm long packed with Pennwatt 223 and 4 percent KOH on an inert support phase manufactured by Applied Science Laboratories, Inc. was used. All sample injections were two microliters from a five microliter syringe from Hamilton.

Before the calibrations of the integrator, the "START DELAY" on the integrator was used to omit the solvent peaks. The feed sample was injected and an "EXTERNAL METHOD" of calibration was

used and each subsequent sample was calculated based on the feed calibration. The external method of calculation was used since constant sample volume was used for the purpose of reproducibility (H.P. Laboratory Automation Products, Instrument Manual, model 3380, 1978).

Based on the above calibration, the ratios of the percent of the component peaks in any given product sample to the percent of the corresponding peaks in the feed sample was obtained directly.

Amount of A in sample product =

$$\frac{\text{Area of A in sample product} \cdot \text{Amount of A in Feed}}{\text{Area of A in feed}} \cdot \text{XF}$$

where XF is a multiplying factor. In all analysis, the value of XF was taken as unity.

CHAPTER 8

RESULTS AND DISCUSSION

The discussion of all results will be offered under three classifications, viz. concentration histories of breakthrough and desorption of column operation using standard elution technology, one and two column parametric pumping, and one and multicolumn staged sequence cyclic process.

DESIGN OF FIXED-BEDS BY THE PREDICTION OF BREAKTHROUGH AND DESORPTION CURVES

An efficient design of a fixed bed adsorption column requires an effective predictive tool of the breakthrough and desorption concentration histories. Problems most often encountered could exhibit favorable or unfavorable nonlinear or linear equilibria. The adsorption and desorption of most organic materials are such that favorable and unfavorable equilibrium isotherms respectively predominate.

Figures 8.1 through 8.3 exemplify the conditions under which unfavorable equilibrium for the system O-Xylene-Anisole-n-heptane in silica gel are obtained. For these desorption cycles proportional pattern behavior of the fluid concentration at the bed exit is achieved. Therefore accurate prediction of the breakthrough of the fluid concentration from these equilibrium behavior and proportional pattern behavior can be obtained. In parametric pumping operation, in short any cyclic operation, and

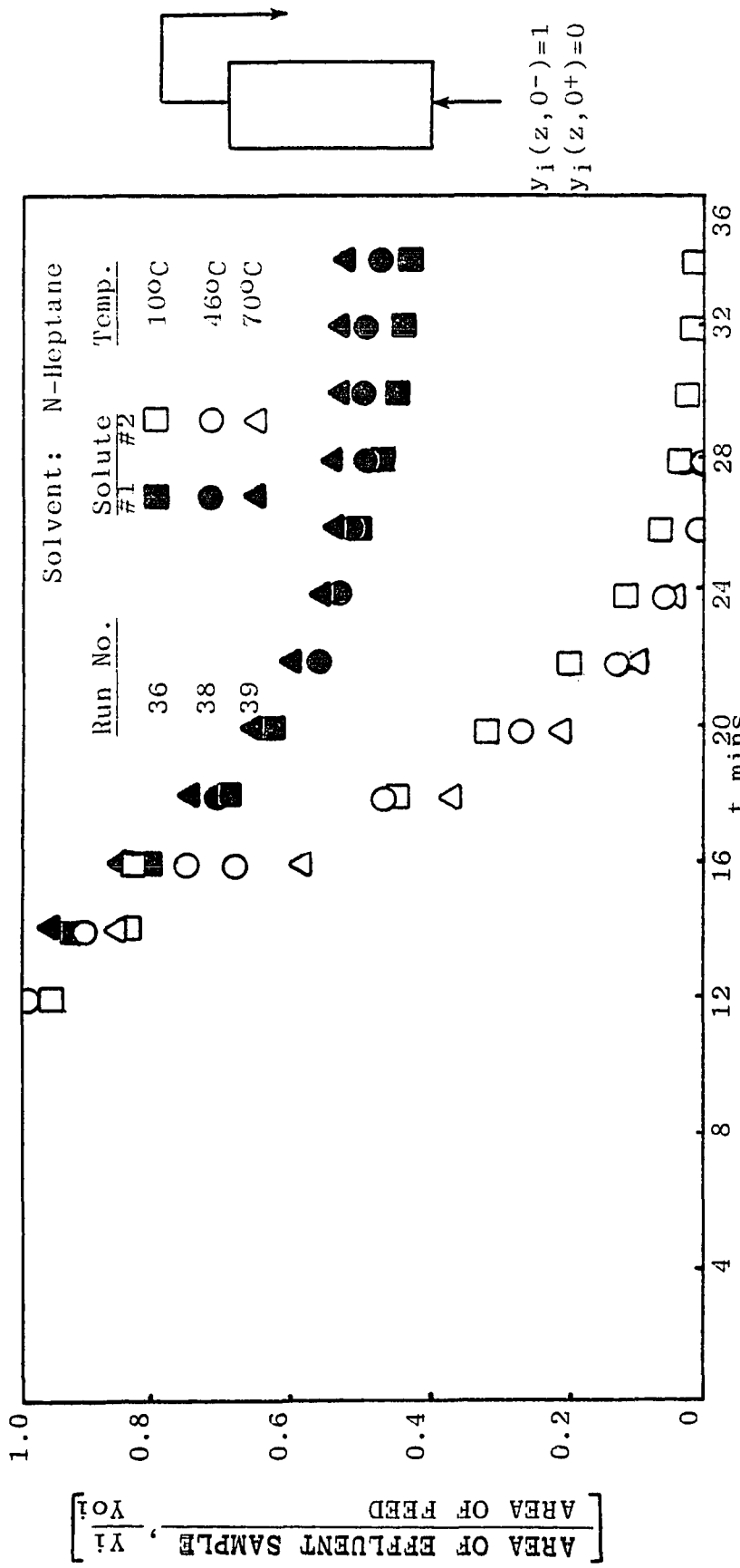


FIGURE 8.1 UNFAVORABLE DESORPTION ISOTHERM FOR O-XYLENE AND ANISOLE COLUMN INITIALLY SATURATED WITH 5% V/V TOLUENE AND 5% V/V ANISOLE IN N-HEPTANE
#1: ANISOLE; #2: O-XYLENE

especially those that involve physical adsorption, desorption is generally the rate limiting step. Figure 8.1 depicts the unfavorable equilibrium relationship for the desorption of 5% v/v O-xylene and 5% v/v anisole in the solvent n-heptane. The unfavorable isotherms for both O-xylene and anisole exhibit a proportionate pattern. The curvatures show no significant difference even at high temperatures. This observation seems to suggest that, at high concentration where the isotherms show no real difference, the driving force (the adsorbed phase concentration difference at the operating temperatures) necessary for a cyclic separation is at a bare minimum and therefore poor separation would result, and in order to achieve a reasonable separation, long cycle time or large numbers of separation stages would be required. The effluent concentration of O-xylene is reduced essentially to zero in about 14-16 minutes or corresponding to 28-32 cubic centimeters of desorbing fluid for the systems employed. On the other hand, the concentration of anisole shows excessive tailing which is indicative of chemisorption. This condition can generally be attributed to the polar character of anisole, hence anisole or polar solutes will not move rapidly especially on polar adsorbents. The nature of the adsorbent account for the mass action equilibria in the cyclic process. Silica gel contains a large variety of active sites, hence polar solutes would exhibit considerable tailing.

Ultimately, the separation of components depends on the ratio of the total amount of each solute in the solid phase to

the total amount of each solute in the liquid phase. This ratio, normally called the capacity factor k' , (Introduction to Modern Liquid Chromatography, Snyder and Kirkland) is a function of temperature. However, only a limited functional dependency of k' on temperature is possible (Schmit, et al., 1971), between the limits set by the mobile phase volatilization point on the upper end and excessive solvent viscosity at lower temperatures. Therefore presaturating the column with O-xylene and anisole at fairly high concentration before desorption at a temperature range of 10°-70°C, the isotherms may not provide an adequate fundamental driving force necessary for separation, since at temperatures considerably higher would be close to the boiling point of the solvent.

Figure 8.2 shows a desorption isotherm for a column presaturated with 1% v/v O-xylene and 1% v/v anisole at temperatures of 30°, 60° and 85°C. The curves for the dilute sorbate concentrations exhibit considerable driving force compared with Figure 8.1. However, examination of the isotherms show that the rate at which the concentration of O-xylene approach zero is higher at high temperatures, while the opposite is the case for the rate at which the concentration of anisole approaches zero. In other words, the velocity, u_i , or the relative frontal movement (RF) for the desorption process,

$$u_{\text{O-xylene}}(T=85^{\circ}\text{C}) > u_{\text{O-xylene}}(T=60^{\circ}\text{C}) > u_{\text{O-xylene}}(T=30^{\circ}\text{C})$$

and

$$u_{\text{anisole}}(T=85^{\circ}\text{C}) < u_{\text{anisole}}(T=60^{\circ}\text{C}) < u_{\text{anisole}}(T=30^{\circ}\text{C})$$

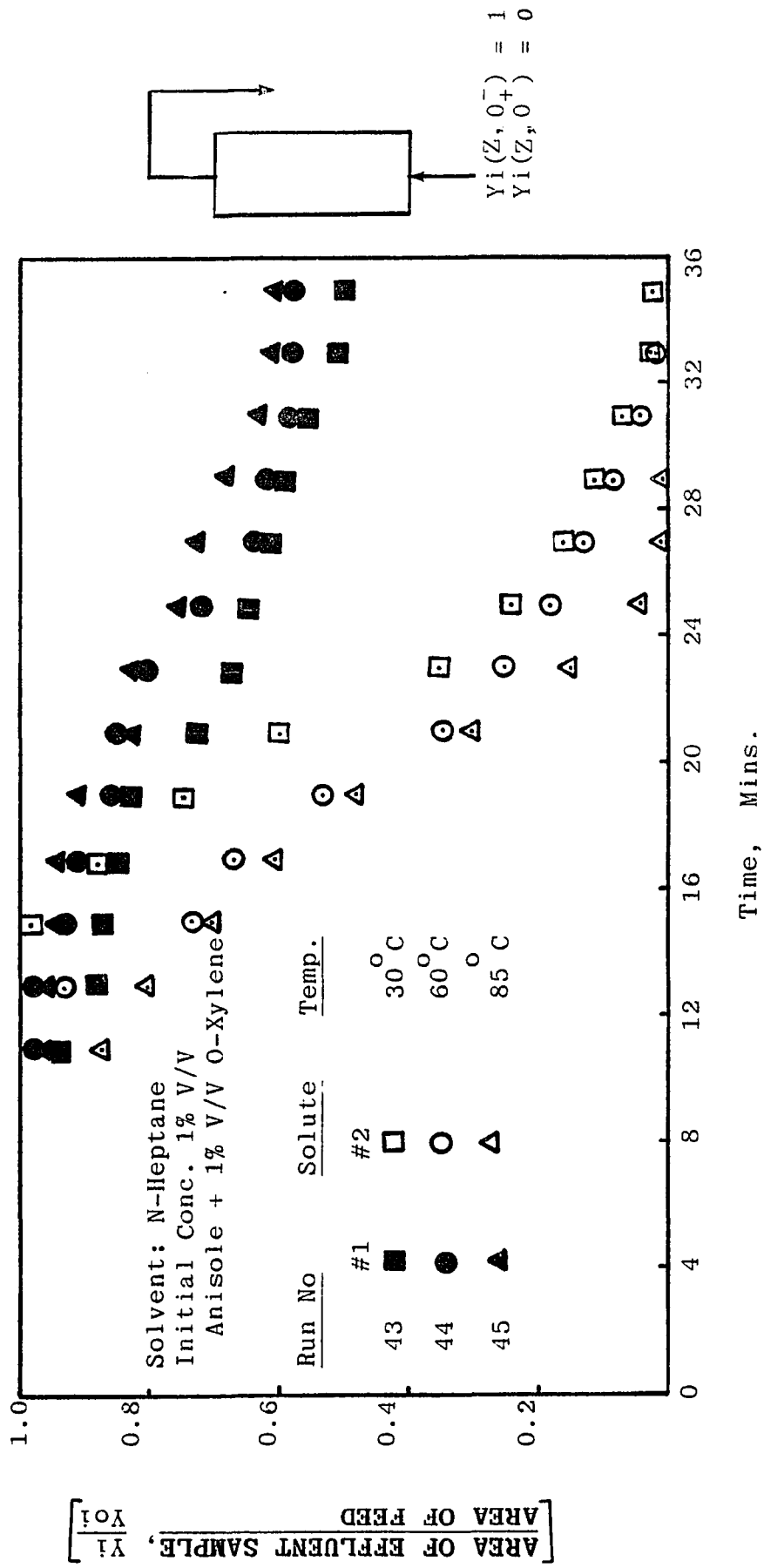


FIGURE 8.2 UNFAVORABLE DESORPTION ISOTHERM FOR O-XYLENE AND ANISOLE

A plausible explanation to this observation is that there is interdependence of the equilibrium distributions of the two species. That is to say that the stationary phase concentration of O-xylene depends not only on the liquid phase concentration of O-xylene, but also on the concentration of anisole, or

$$x = f(\text{O-xylene, Anisole}) \text{ (in equilibrium)}$$

This would also mean that there is competition between O-xylene and anisole for the limited number of adsorption sites of silica gel. The velocity of O-xylene ($u_{\text{O-xylene}}$) increases with increase in temperature thereby depleting the concentration of O-xylene in the solid phase. By so doing, there is less competition for anisole and its concentration in the solid phase is increased with a decrease in O-xylene concentration. This phenomena would lead to the conclusion that molecules with higher affinity provide stronger competition and therefore greater reduction of the solid phase concentration. One could also conclude that with increase in temperature, the velocities of molecules with lower affinity will be higher than the velocities (RF) of molecules with higher affinity.

From the desorption curves shown so far (Figures 8.1 and 8.2), the excessive tailing of anisole is observed. For efficient design of cyclic process (adsorption and desorption), it would, of course, be desirable to reduce all effluent concentrations to some arbitrary value close to zero, especially with an increase in temperature. Since the upper limit of the temperature that could be used is set by the boiling point of the

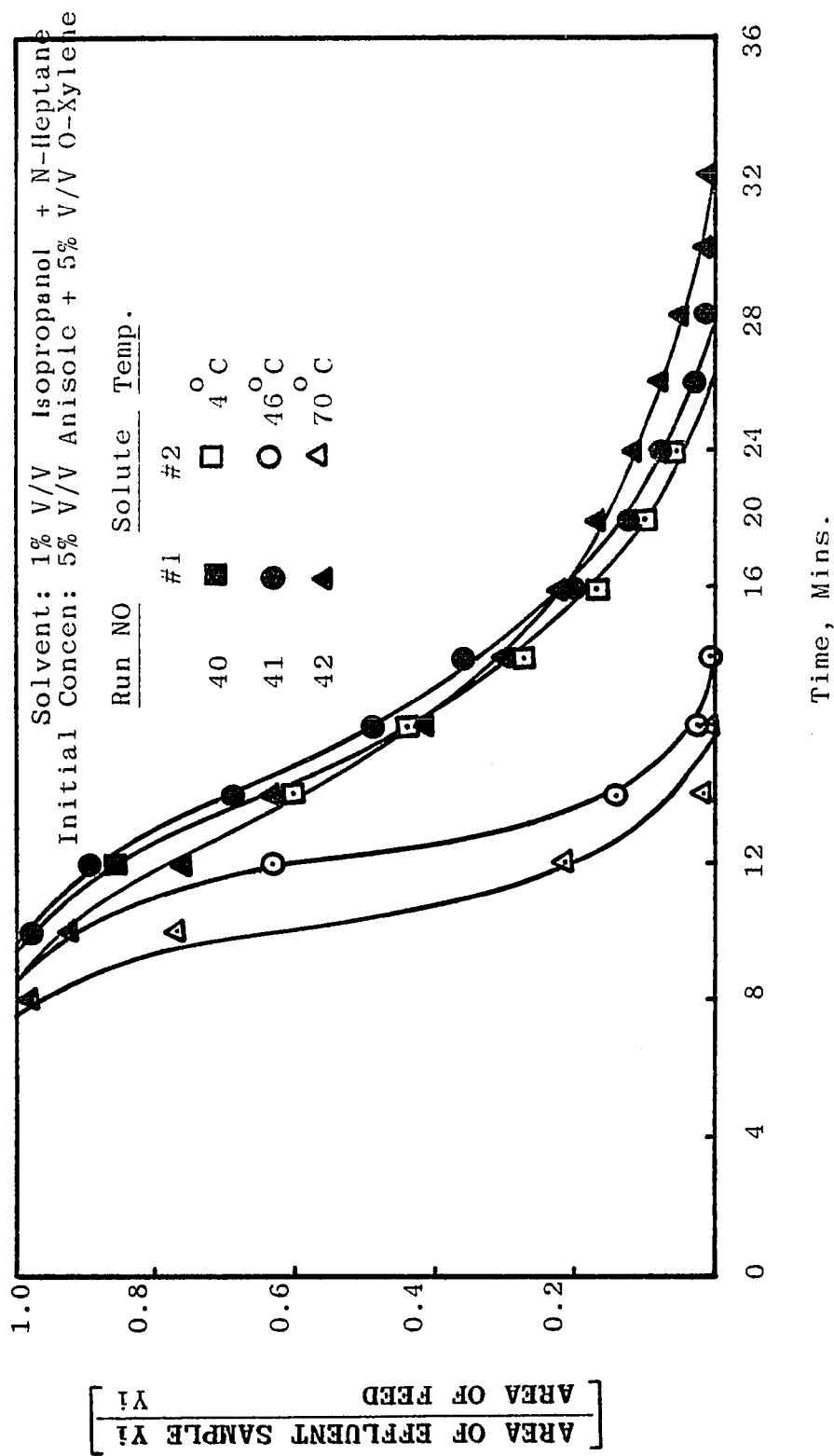


FIGURE 8.3 EFFECT OF SOLVENT MIXTURES ON DESORPTION OF O-XYLENE AND ANISOLE

#1: ANISOLE #2: O-XYLENE

solvent, a mixture of two solvents such as polar and nonpolar solvents (e.g. heptane and isopropanol) would reduce this tailing effect. Figure 8.3 shows desorption curves with a mixture of two solvents, n-heptane and 1% v/v isopropanol. Although the tailing effect has been successfully reduced, the isotherms over the temperature range show no measurable driving force necessary for effective cyclic separation. Since there is no significant difference in the curves for a given solute at all temperatures, it would be reasonable to assume that temperature will not be an effective cyclic variable when a mixture of two or more solvents are used. A mixture of nonpolar solvent and a concentration of a polar solvent below 1% v/v would result in demixing (Introduction to Modern Liquid Chromatography, Snyder and Kirkland), and above 1% v/v no retention of O-xylene and anisole is observed, i.e. the solid phase concentration of both solutes rapidly approaches zero after the addition of approximately one void volume of desorbing solvent, thereby reducing the rate of mass transfer between the solutes and the adsorbents considerably.

Figures 8.4 through 8.7 show major functional diagrams obtained from the breakthrough patterns based on Eq. 3.86. The expression of Eq. 3.86 is based on the premise that in the rate expression transport resistances in the fluid phase around the particles dominate. However, this equation (Eq. 3.86) is an approximation for estimating breakthrough curves in that it does not account for all necessary transport resistances in the solid

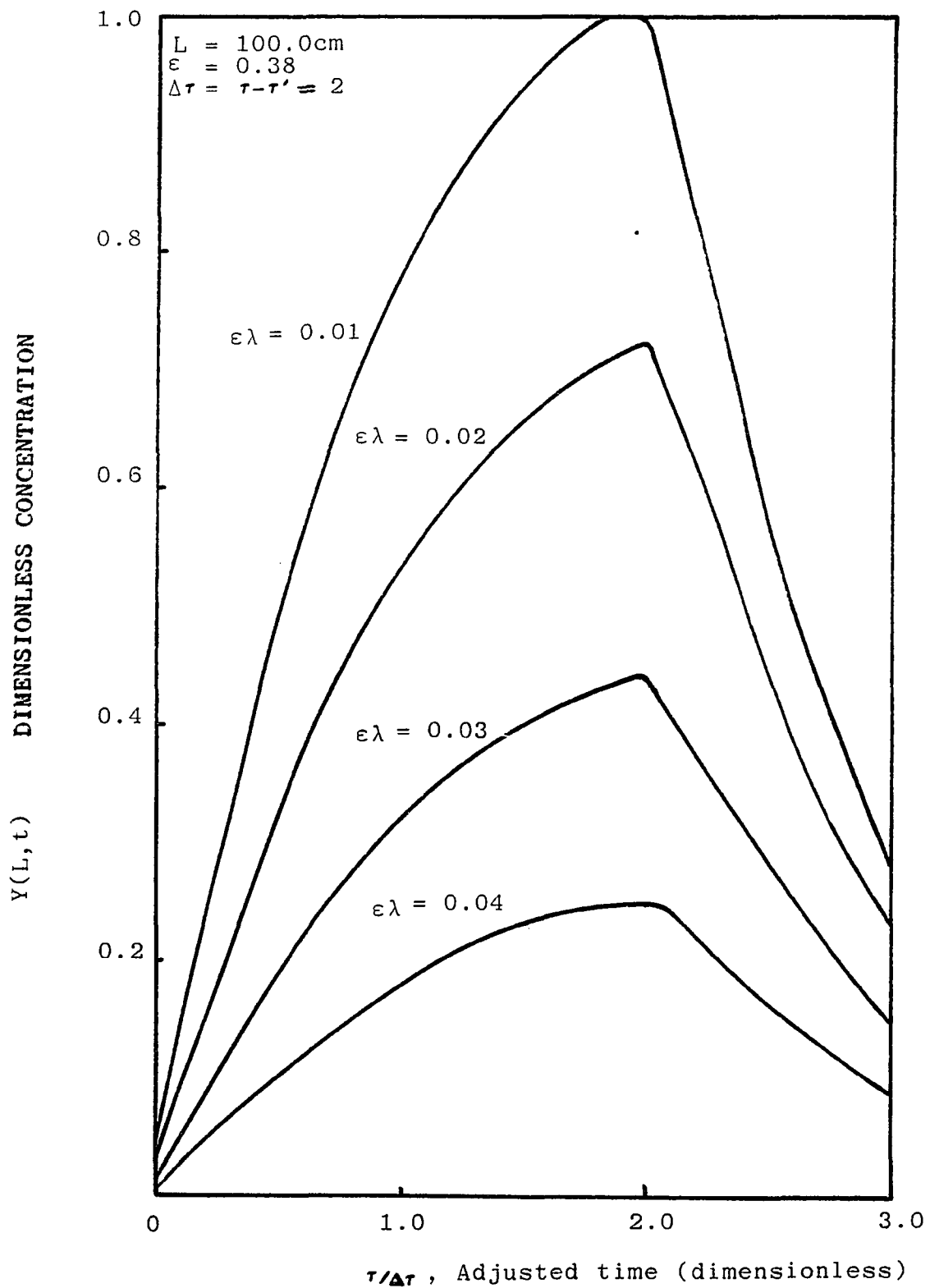


FIGURE 8.4 CONCENTRATION - TIME DIAGRAM FOR VARIOUS MASS TRANSFER COEFFICIENT

and fluid phase. For precise determination of breakthrough curves, Eq. 3.49 should be used. Equation 3.49, even though the derivation was based on linear equilibrium instead of the more realistic nonlinear equilibria, precisely accounts for the unsteady state diffusion in the solid and liquid phases, and all of the various transport effects. Even though this complete model equation for a packed bed accounts for all the dispersive tendencies, in practice it is rather cumbersome to use. Equation 3.86 presents a very useful simplification, therefore all breakthrough curves were obtained via this simplified form.

Figure 8.4 shows the effluent concentration as a function of reduced time for various mass transfer coefficient. The rear flanks of the curves exhibit well dispersed gaussian type curves, but the shape of the latter portion of the effluent curves show a nongaussian type distribution. As the column is being loaded, the solute spreads out as it moves with the solvent down the column because of dispersion. The amount of spread depends on the intensity of the dispersive forces. However, as soon as the introduction of pure solvent is begun, the spread is reduced, and thus the dispersive phenomena, hence the curves are nonsymmetrical. It can also be seen that the sharpness of the curves decrease with an increase in mass transfer coefficient. At slow mass exchange, the peaks are sharp and tall, an indication of unretained solute, and as mass exchange is increased, the solutes are gradually retained and the peak shape becomes broader with decreasing height.

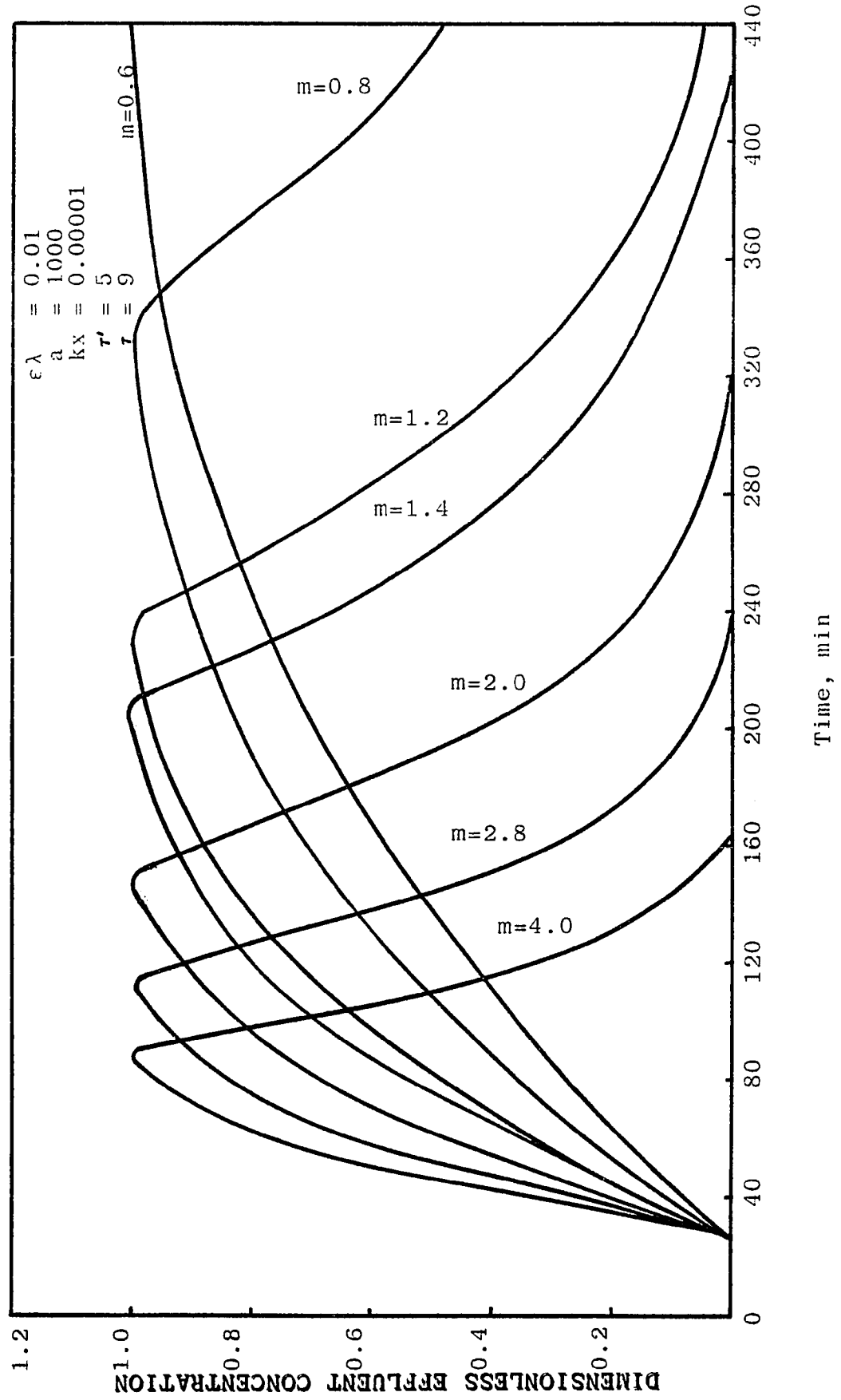


FIGURE 8.5 CONCENTRATION-TIME DIAGRAM FOR VARIOUS EQUILIBRIUM CONSTANTS

Figure 8.5 illustrates a series of concentration-time curves for various equilibrium constants. This figure exemplifies the characteristic behavior of linear systems, as the effluent concentration distribution remains constant for all ranges of equilibrium constants. The peaks become sharper with an increase in equilibrium constant. These simplistic behavior which is characteristic of linear systems are widely responsible for the wide usage and application to fixed-bed separation processes.

Figures 8.6 and 8.7 show the dimensionless effluent concentration profile as a function of equilibrium constants for fixed values of t for both adsorption and desorption steps. From Figure 8.6, it can be seen that for $m < 1.3$ for a column of 100 cm in length, the slope of the adsorption step at 80 minutes exhibits a linear relationship, while the desorption at 200 minutes exhibits a near nonlinear relationship.

For the adsorption step and for $m > 1.3$, the slope is nonlinear and approaches the maximum dimensionless concentration of unity while the concentration of the desorption step goes through a maximum concentration of unity and then suddenly decreases in a nonlinear fashion. The sudden decrease is a consequence of the fact that as the equilibrium constant increases, the fluid phase concentration is quickly depleted for a fixed time ($k \rightarrow \infty$, $y \rightarrow 0$ for a given t). Figure 8.7 shows the case for which $0.1 \leq m \leq 1.0$ for both the adsorption and desorption steps at 60 and 200 minutes respectively for column lengths of 5, 25 and 50 centimeters. For

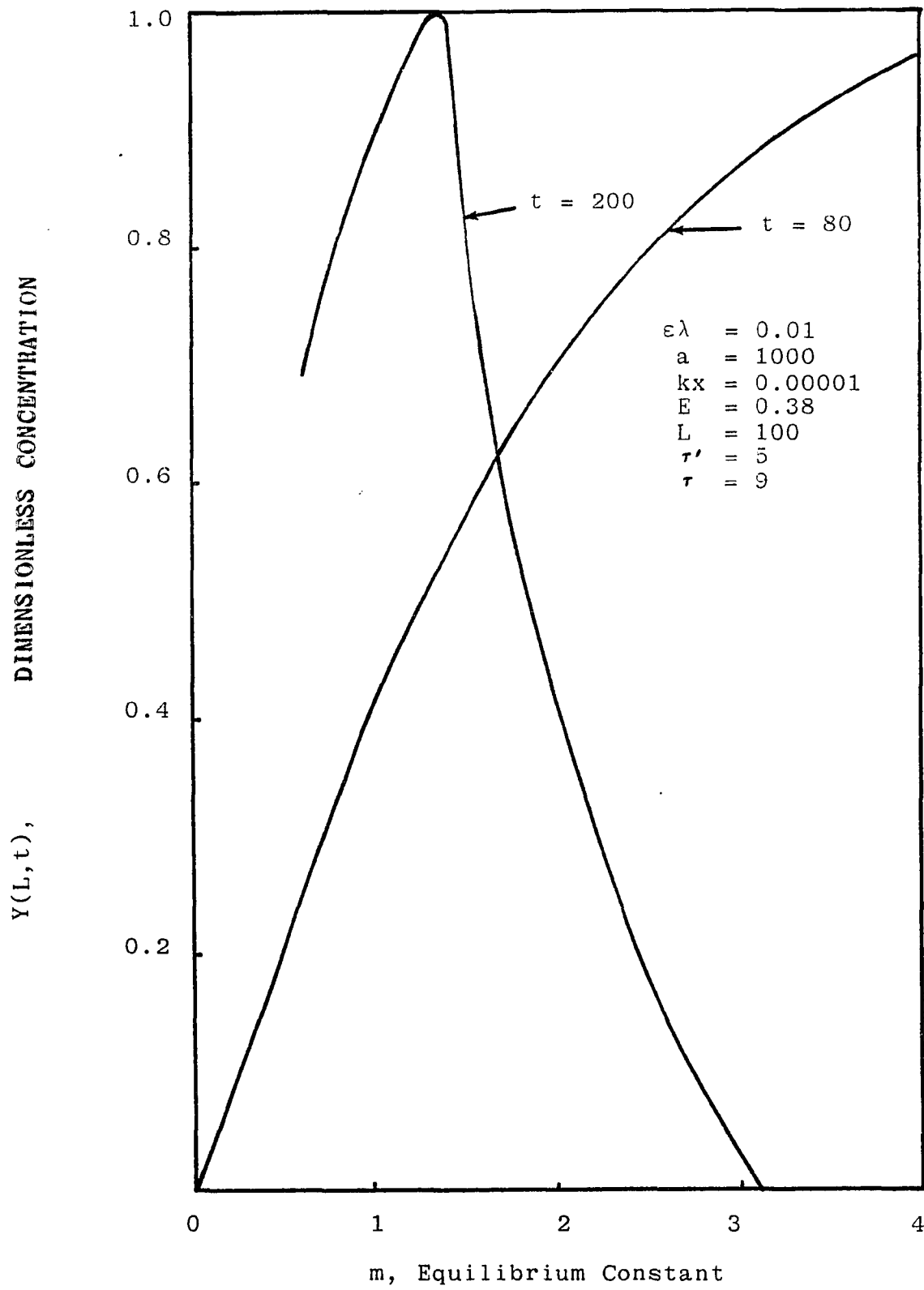
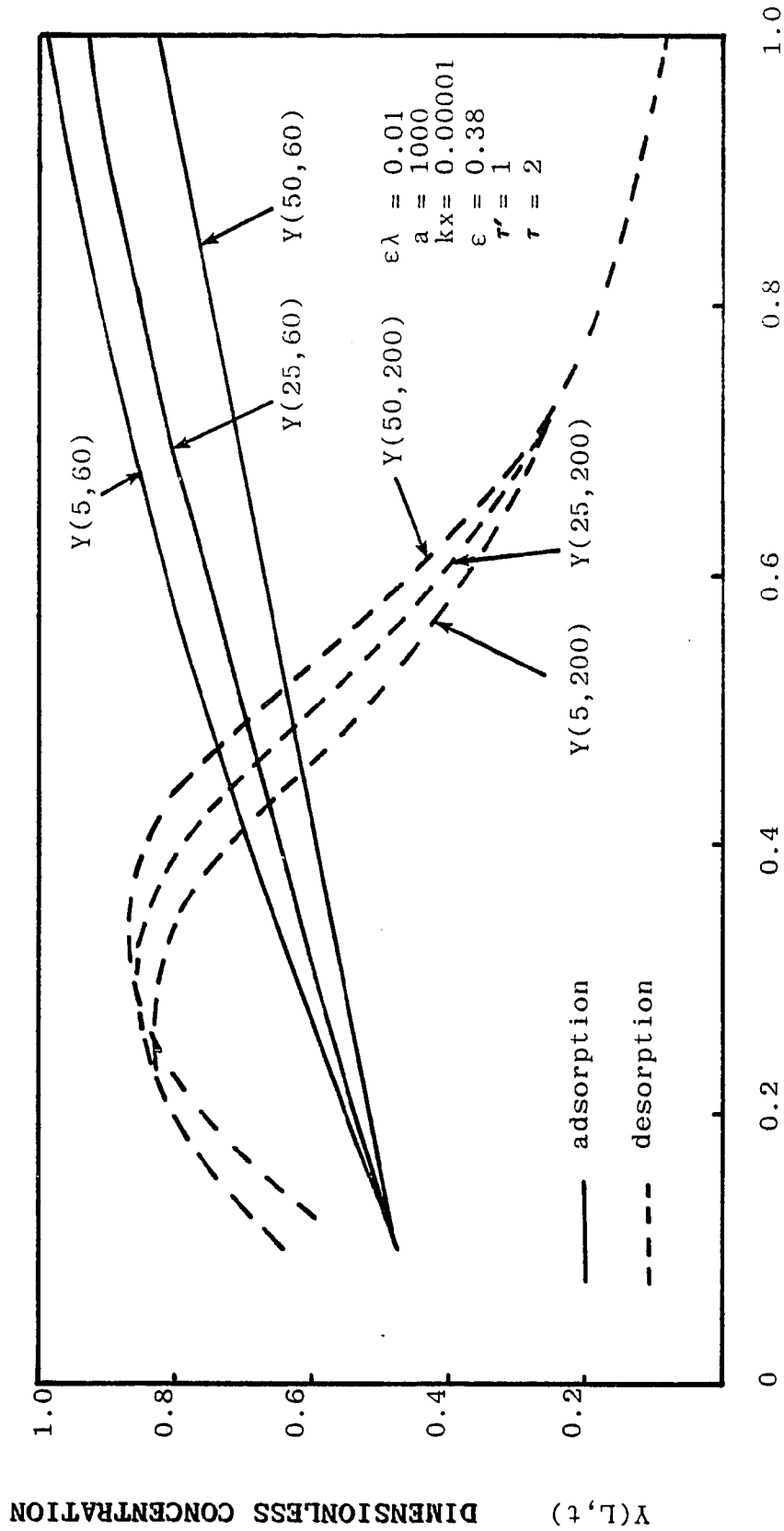


FIGURE 8.6 EFFECT OF EQUILIBRIUM CONSTANT ON EFFLUENT CONCENTRATION



the adsorption step, the effluent concentrations approach unity very gradually with increase in column lengths. As $m \rightarrow 0.1$, the effluent concentrations tend towards a focal point for all column lengths. The desorption step curve generated at $t=200$ minutes also shows a maximum, and as $m \rightarrow 1$, the three curves degenerate toward a focal point and further toward an asymptote

PARAMETRIC PUMPING

All one column parametric pumping runs were performed with 2.5 volume percent toluene and acetophenone in n-heptane (dilute solution, Stokes (1976)). A total of ten runs with a single column configuration either operating in a top or bottom feed mode (Chen, 1971, 1972, 1973, 1974) are presented. Pertinent operating variables necessary for the operation of a two column configuration were optimized with the one column process. Six runs performed with a two column configuration are also presented. The complete experimental data for one and two column parametric pumping are shown in tabular form in Appendices II and III respectively. Some of the data are plotted as product/feed solute concentration ratios or percent recovery versus number of cycles, n . The column/columns were operated between temperature levels of 298°K (25°C) and 343°K (70°C), the ratio of the feed to reservoir volume ranged from 0.1 to 0.4, and the top and bottom reservoir dead volumes were 5 cubic centimeters. The one column dimensions are 1.0 cm in diameter and 90 cm in length glass column, and the two column parapump consisted of stainless steel columns of the same dimensions.

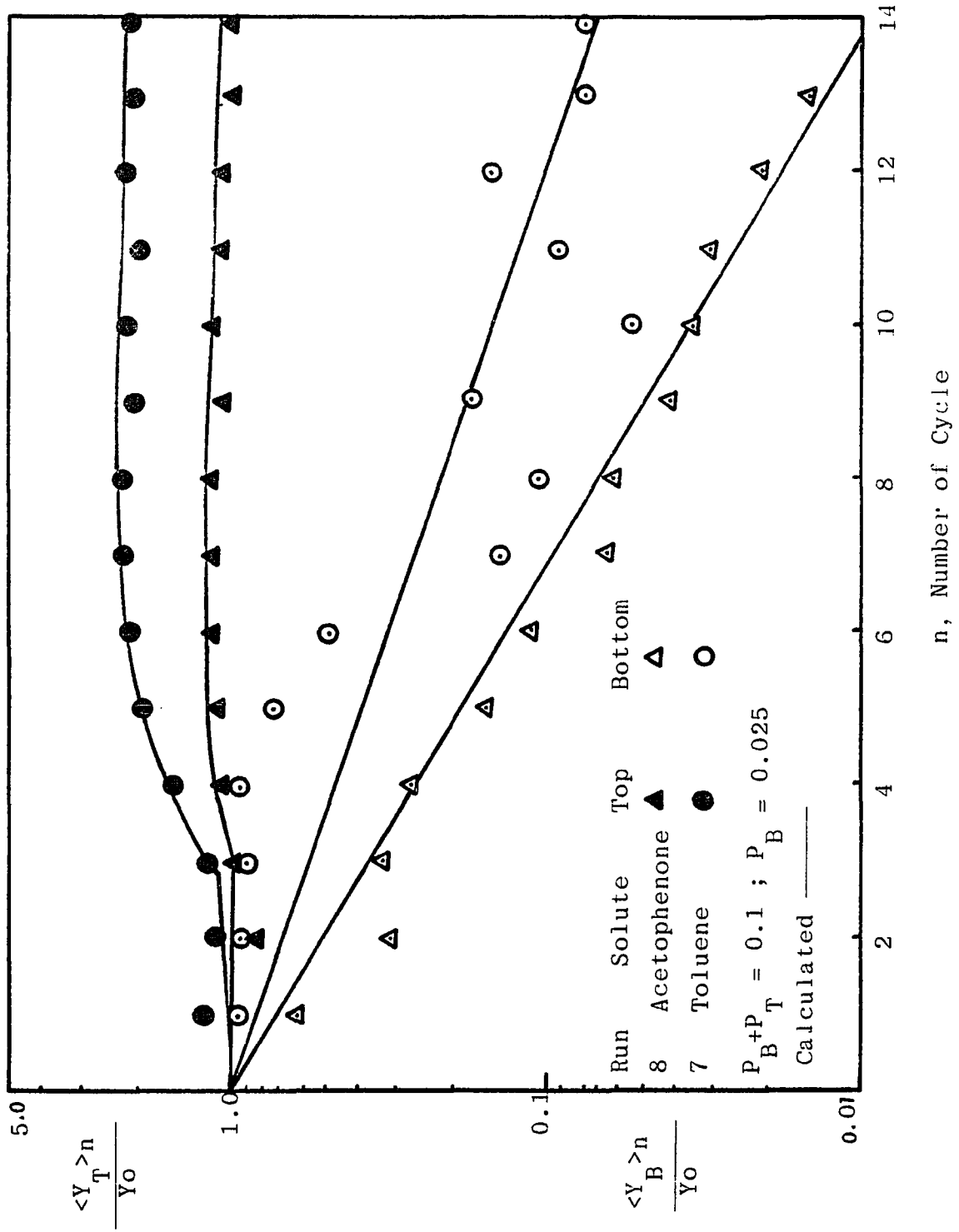


FIGURE 8.8 ONE COLUMN SEMI CONTINUOUS PARAPUMP WITH TOP FEED

Figures 8.8 through 8.10 illustrate the separation attained with a one-column semicontinuous parapump with top feed for values of top and bottom product withdrawal rate (P_T+P_B) operated at half cycle time of 20 minutes. One can see from Figure 8.8 that the transients for depletion of the bottom product, $\langle y_B \rangle_n / y_0$ is more gradual compared to that in Figure 8.9. Therefore it is clear that the transient times to remove the solute from the bottom reservoir or the bottom product stream is long. At steady state, however, $\langle y_B \rangle_\infty / y_0$ for $P_T+P_B=0.1$ and 0.25 would be approximately equal. Figure 8.10 shows a case for $P_T+P_B=0.40$, which would correspond to feed of 16cc over the entire half cycle time since the reservoir displacement is 40 cc. The separation obtained is poor because more product is withdrawn per half cycle, and a build up of dilute solution is prevented. The separation improves with a decreasing P_T+P_B and, as P_T+P_B becomes smaller, conditions of close parametric pump or batch pump is approached (Chen, 1971). Based on equilibrium theory, Chen et al. (1974) predicted that there exists an optimal reservoir displacement flow rate Q_{max} and an optimal bottom product flow rate $P_{B_{max}}$, of which the bottom product concentrations, $\langle y_B \rangle_n / y_0$ decreases as n increases for a parapump operated in a semicontinuous mode as long as $Q \leq Q_{max}$ (or $Q t \leq Q_{max} t$) and $P_B \leq P_{B_{max}}$ (or $P_B t \leq P_{B_{max}} t$) and t being the half cycle time. The above conditions are necessary conditions for a monotonically decreasing bottom product concentration. For all runs, $Q_{max} t \approx 40.0$ cc and $P_{B_{max}} \approx 0.9$ ($P_{B_{max}} = Q_{max} (2b/(1-b))_k$). In Figure 8.8 for which $P_B = 1.0$ the monotonic decrement of the

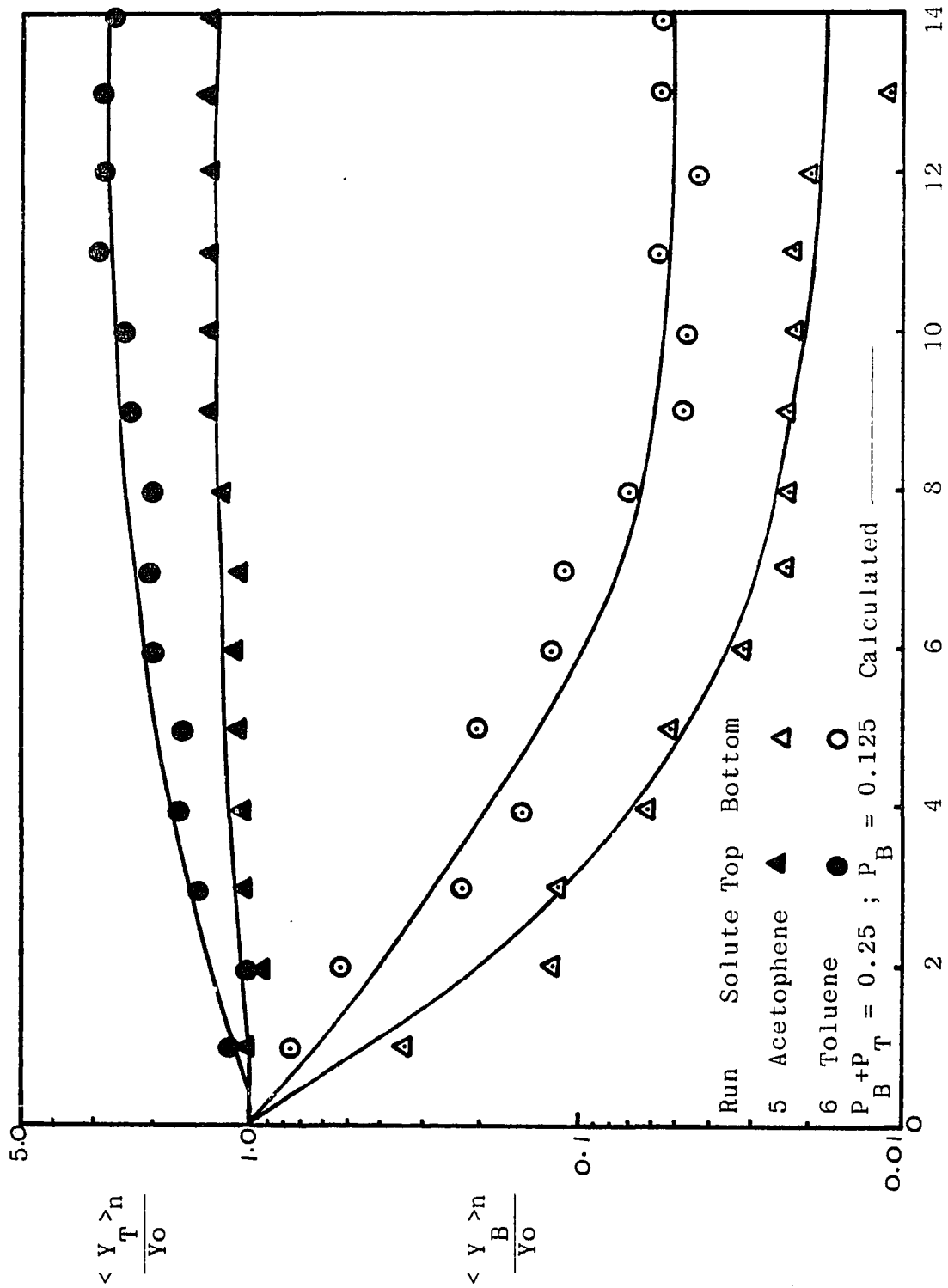


FIGURE 8.9 ONE COLUMN SEMI CONTINUOUS PARAPUMP WITH TOP FEED

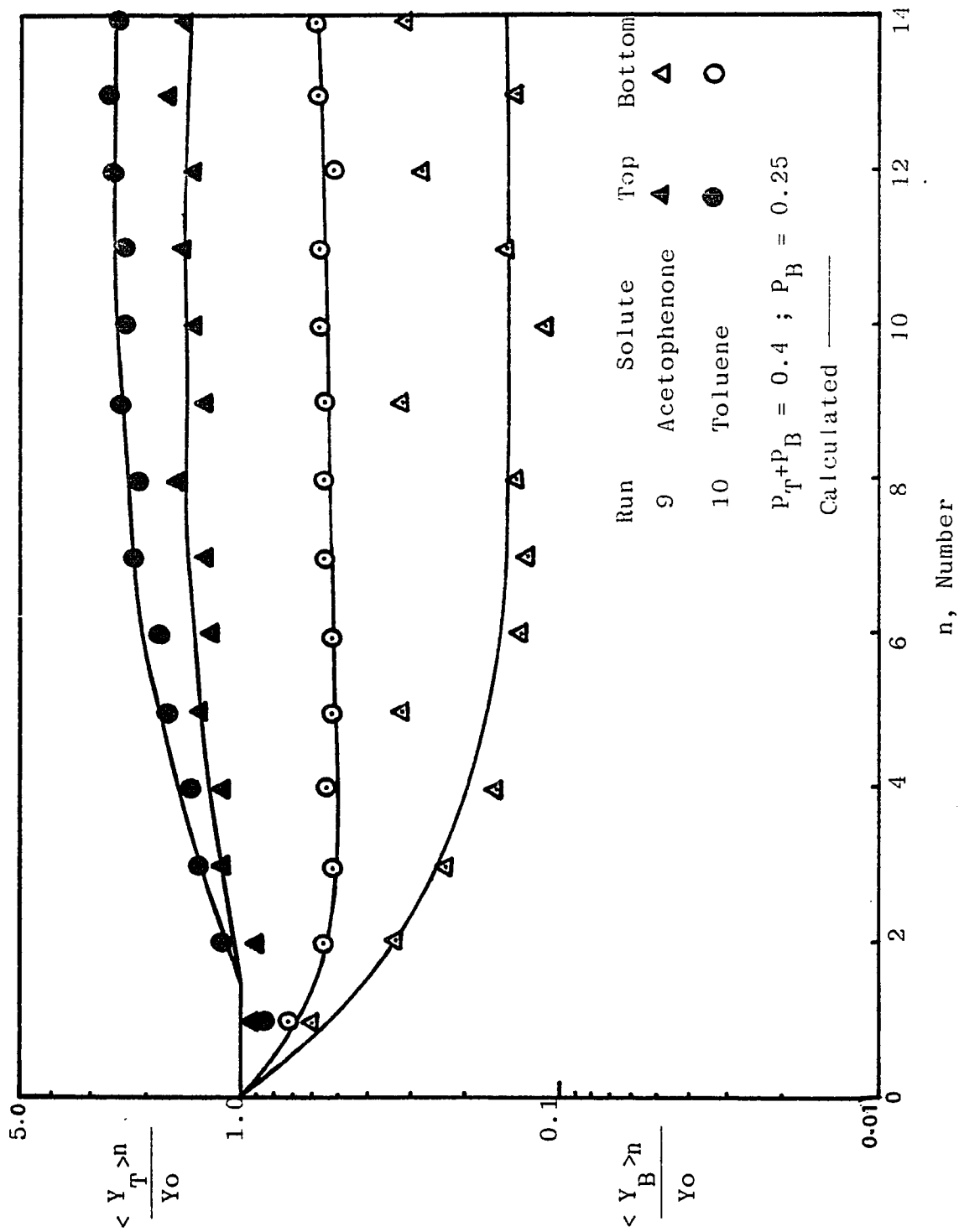


FIGURE 8.10 ONE COLUMN SEMICONTINUOUS PARAPUMP WITH TOP FEED

bottom product can be seen, but Figures 8.9 and 8.10 with $P_B=2.5$ and 5 respectively, where $P_B > P_{B_{max}}$, the steady state behavior switches from a situation of which the solutes are completely removed from the bottom reservoir to one in which the solute removal is incomplete.

Figures 8.11 and 8.12 illustrate the effect of the feed location (top or bottom feed) on the concentration transients for a continuous parapump operation. Figure 8.11 shows an initial downward slope of the acetophenone bottom product stream, it extends to the fifth cycle and is followed by an upward turn to the eighth cycle and levels off after cycle number 8. This dip was not observed in the semicontinuous runs, even over the wide range of P_T+P_B employed. Stokes (1976) observed similar experimental results, but contended that the dip was sensitive to the value of the bottom product withdrawal rate (P_B). Similar phenomena (Fig. 8.11) was observed with toluene but less pronounced. Figure 8.12 shows the concentration transients for the continuous pump with bottom feed. Chen and Hill (1971a) in the analysis of the performance characteristics showed that a continuous pump will produce bottom solute concentration with incomplete solute removal for certain values of P_B compared with a semicontinuous pump where complete solute removal is possible. This observation is a consequence of the loci of switching points between Region 1 [$L(T_1) \leq L(T_2)$ and h_{c01}] and Region 2 [$L(T_2) < L(T_1)$ and $L(T_2) \leq h_{c01}$] for which $P_B = 2b/(1-b)$ for semicontinuous and $P_B=b$ for a continuous pump. The

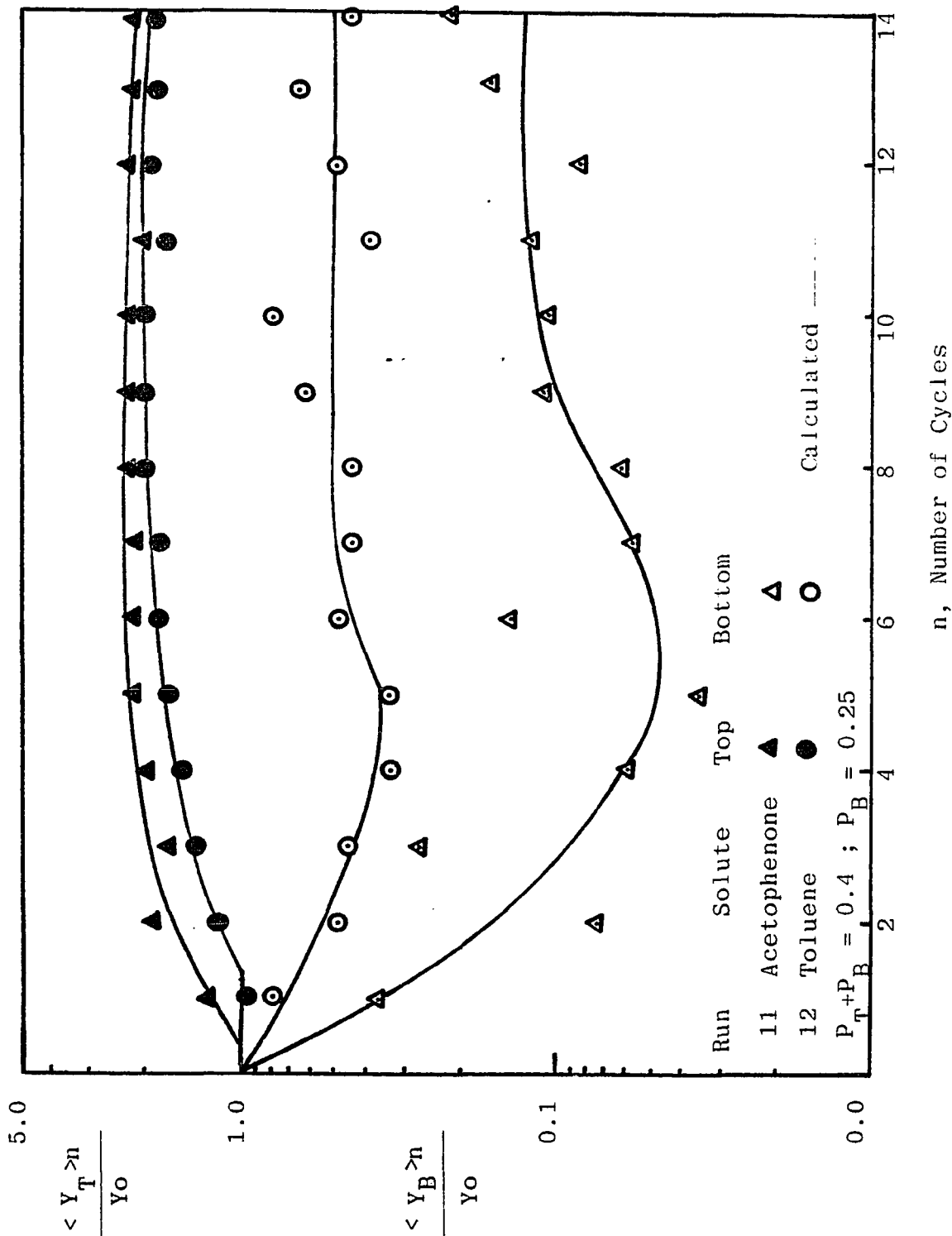


FIGURE 8.11 ONE COLUMN CONTINUOUS PARAPUMP WITH TOP FEED

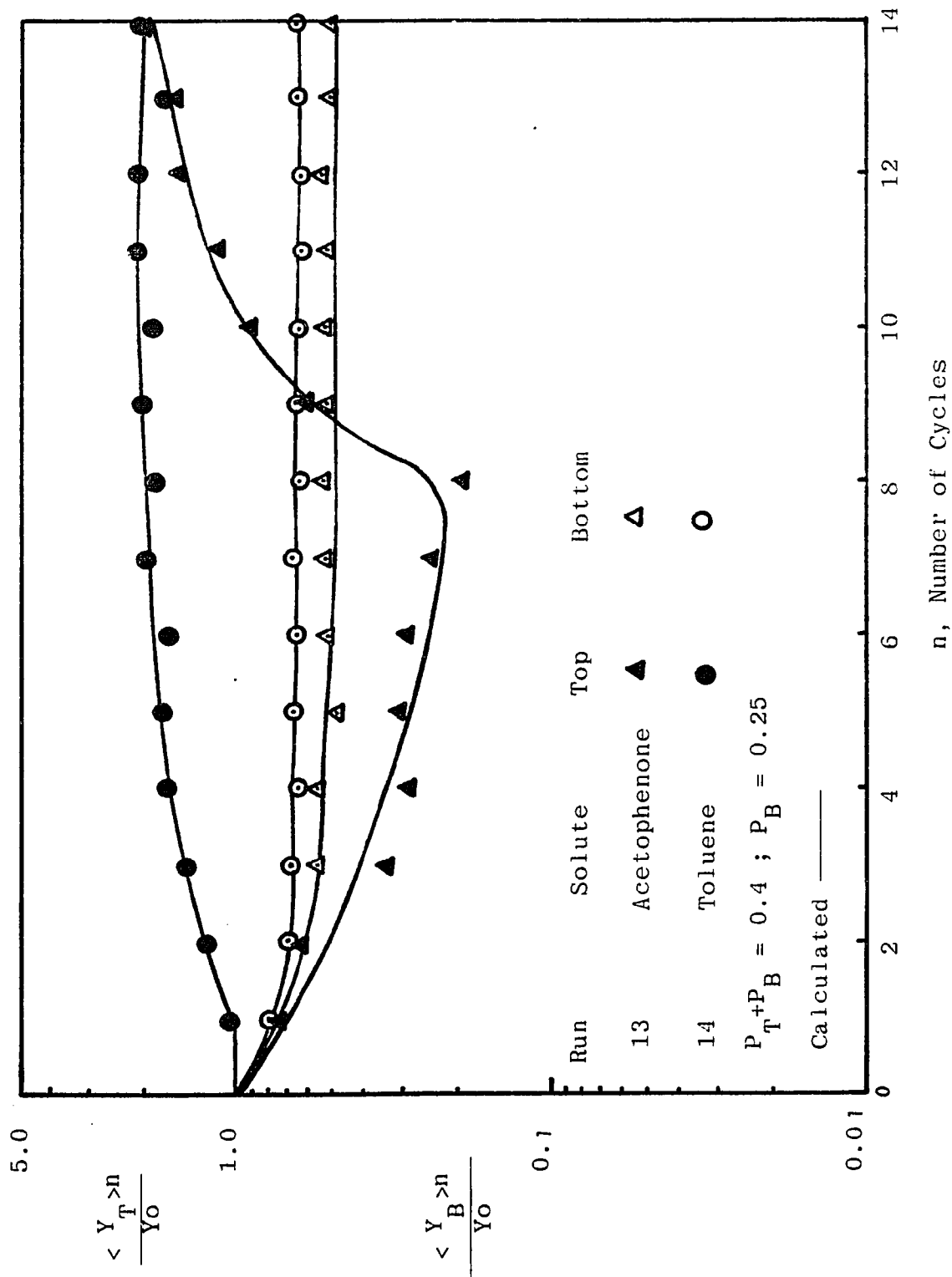


FIGURE 8.12 ONE COLUMN CONTINUOUS PARAPUMP WITH BOTTOM FEED

authors also predicted that the purification of the bottom product achieved with continuous pumps with bottom feed would be considerably less than that achieved with top feed. A comparison of the bottom products (see Figs. 8.11 and 8.12) shows that $\langle y_B \rangle_\infty / y_O$ (top feed) is less than $\langle y_B \rangle_\infty / y_O$ (bottom feed). Figure 8.12 shows a down turn for $\langle y_T \rangle_n / y_O$ with values less than unity for acetophenone up to the eighth cycle followed by a sharp turn upwards to values greater than unity and asymptotically approaching the value of two as observed by the previous runs (Fig. 8.11). One physical interpretation is that the acetophenone initially saturating the entire column is rapidly adsorbed from the solution and the dilute n-heptane solution is displaced down the column by the main stream until the normal acetophenone concentration wave from outer ends breaks through the top of the column at the eighth cycle. Another reason for incomplete removal of solute from the bottom product stream from pumps with bottom feed is because of the introduction of feed at the bottom. The separation factor for this continuous mode of operation can be large for small P_T (Chen and Hill, 1971a).

Figure 8.13 shows the net direction of concentration fronts moving through the column as a function of n for the two column parametric pumping with alternating top and bottom feed. In this figure, the net movement of toluene is in Region 1 (Chen and Hill, 1971a) where $L_{\text{toluene}}(T_2) > L_{\text{toluene}}(T_1)$, while the net movement of acetophenone is in Region 2, where $L_{\text{acetophenone}}(T_1) > L_{\text{acetophenone}}(T_2)$. The two column process arranged back-to-

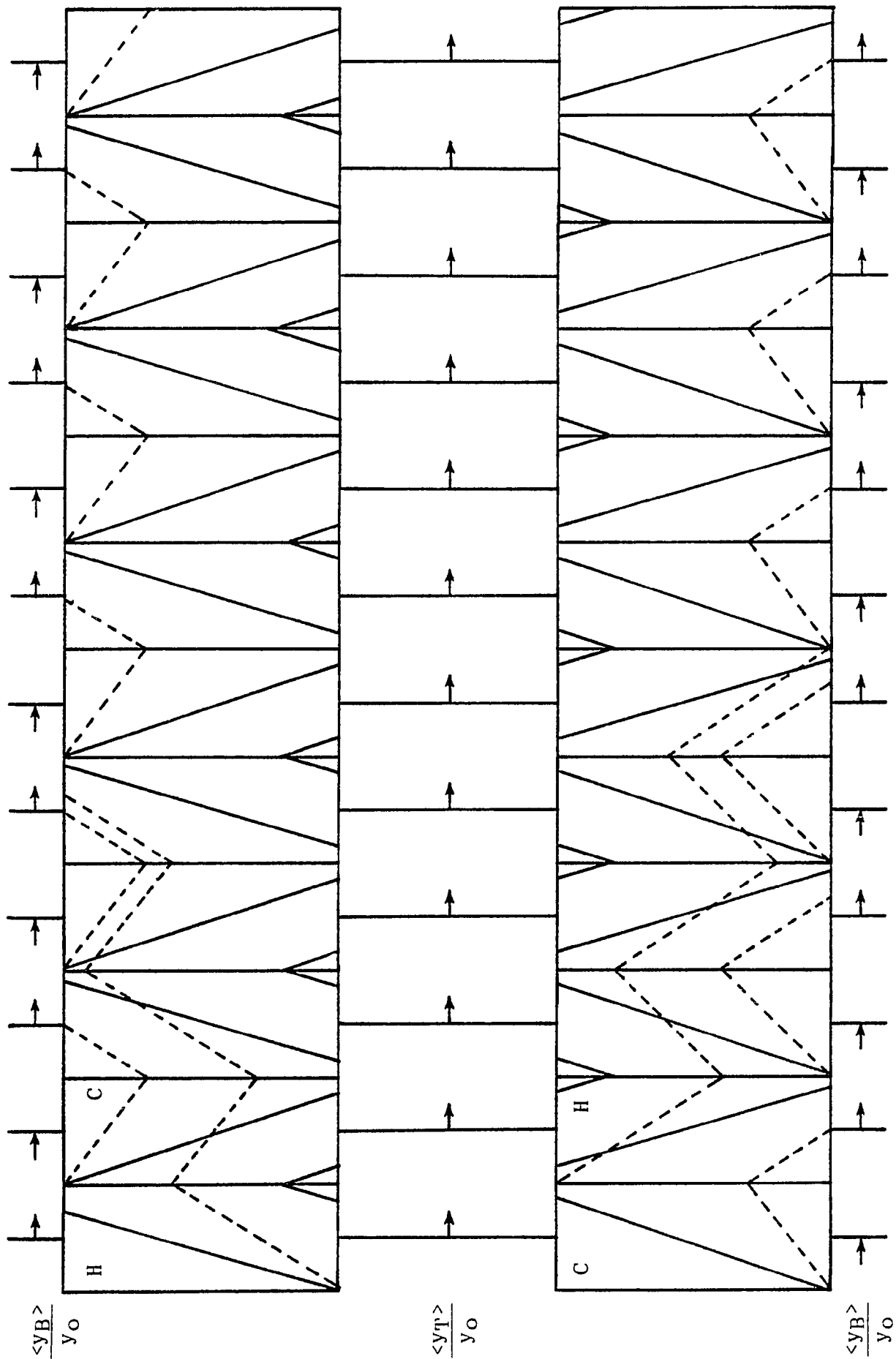


FIGURE 8.13 MULTICOMPONENT WAVE FRONTS FOR OPERATION IN REGIONS 1 AND 2

——— ACETOPHENONE(B), $L_A(T_2) > L_A(T_1)$; $L_B(T_2) > L_B(T_1)$;
 - - - - - TOLUENE(A) $L_A(T) > L_B(T)$

back is a combination of the two modes of column arrangements, viz. top and bottom feed single column process. Thompson and Bowen (1972) in a communication proposed an idealized back-to-back column arrangement that may minimize mixing in a closed (batch) parametric pumping by eliminating reservoirs at the column ends. Though the method of Thompson and Bowen would be experimentally impossible to perform, it does, theoretically, show, however, that the separation factor for the band of the highest concentration is of the order $(\text{constant})^{4n-1}$ for a double column process in the absence of mixing. In Figure 8.13, the pump is operated so that the characteristics of toluene originating from the end of the column at T_1 exit at the inner ends of the column while the characteristics of acetophenone originating from the end of the columns at T_1 do not break through and eventually terminate at the same end at T_2 when the cycle is reversed. Thus, when the mixture is introduced into the columns at T_1 for certain values of P_T and P_B , toluene would leave at the inner ends of the columns and acetophenone would leave at the outer ends with a relative recovery of toluene less or equal to 100 percent, while acetophenone would be considerably less than 100 percent for a feed concentration of 50 percent toluene and 50 percent acetophenone. In the on-going analysis, the effects of P_T and P_B on the steady state characteristics are shown in Figures 8.17 and 8.18.

Figures 8.14 through 8.16 and Figure 8.18 show the effects of feed (P_B+P_T) , and/or top product (P_T) withdrawal rate on

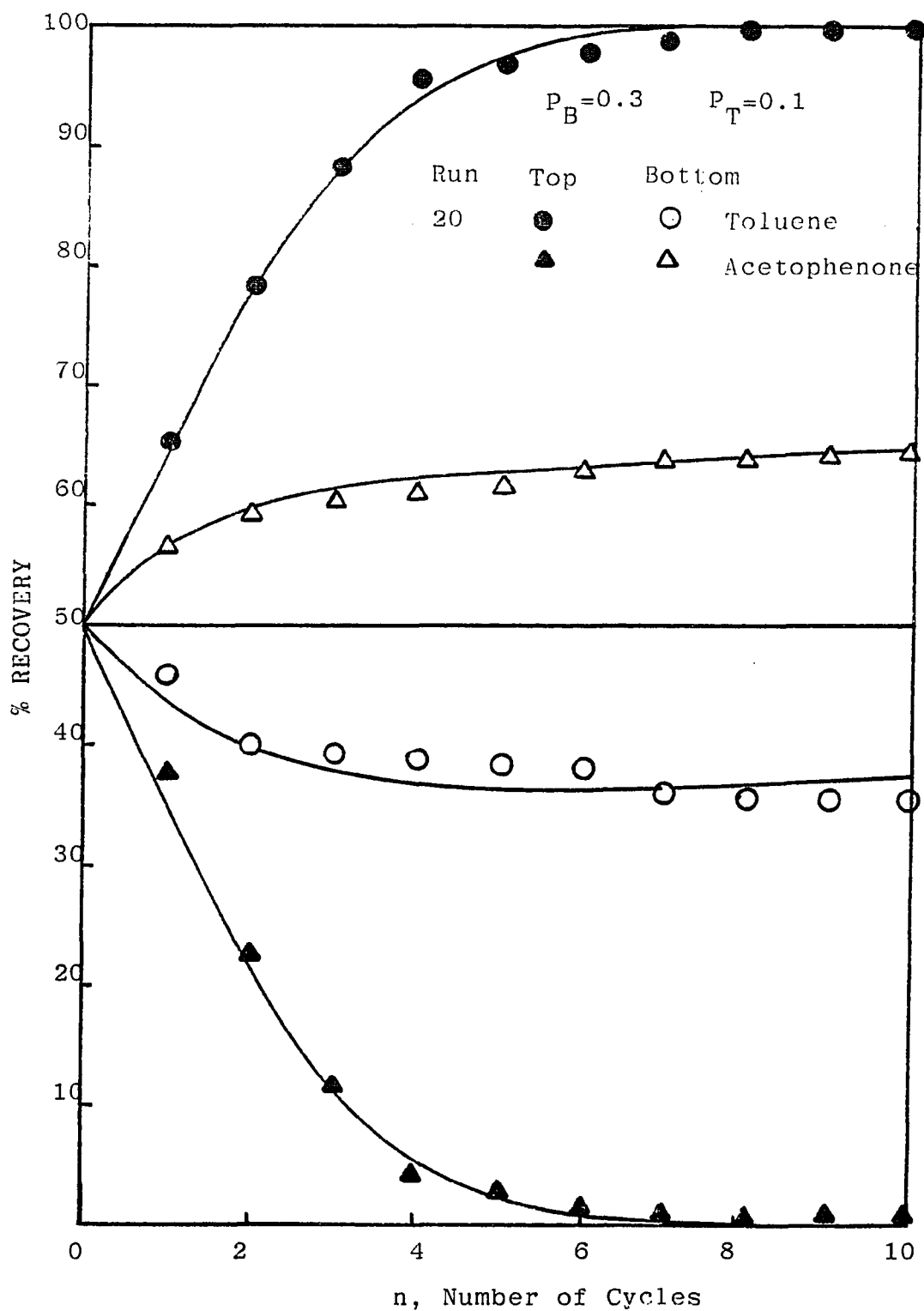


FIGURE 8.14 CONCENTRATION TRANSIENTS FOR $P_T = 0.1$ AND $P_B = 0.3$

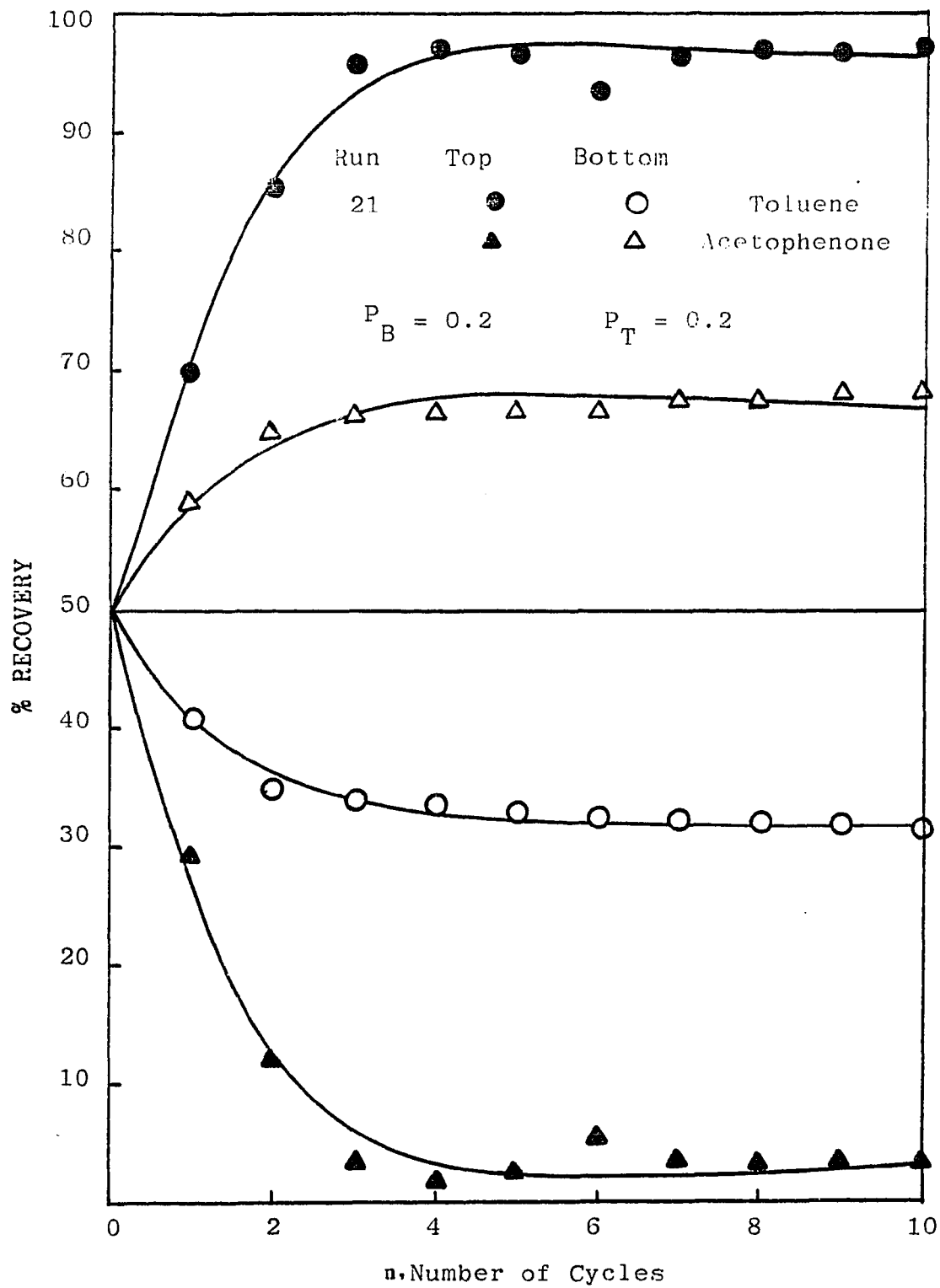


FIGURE 8.15 CONCENTRATION TRANSIENTS FOR $P_T = 0.2$ AND $P_B = 0.2$

percent recovery and the steady state characteristics for toluene and acetophenone for alternating top feed two column parametric pumps. It should be noted, as pointed out in Chapter 6, that of special interest is the top product concentration $(\langle y_T \rangle_n / y_O)$, i.e. effluents leaving the inner ends of the columns where minimum mixing occurs. The bottom product concentration $(\langle y_B \rangle_n / y_O)$ fronts for acetophenone as shown in Figure 8.13 shows no real build up of concentration fronts, partly because the penetration distance of acetophenone when the feed is introduced is much less than the penetration distance for toluene, and when the pumping direction is reversed, some of the acetophenone that accumulated in the previous half cycle is pumped out of the column and a portion is collected as bottom product, while the rest is pumped to the bottom reservoir. Other reasons for the low percent recovery of acetophenone from the bottom product are that tremendous mixing occurs, especially with fresh feed, and mixing decreases separation (Thompson and Bowen, 1972; Wankat, 1978); and from Figures 8.14 through 8.16 and Figure 8.18, it can be seen that the percent recovery of acetophenone steadies out at almost 60% on the third or fourth cycle, which means that acetophenone is partially immobilized on the upper section of the column. The immobilization of acetophenone is a result of chemisorption (Figs. 8.1 and 8.2) since the bulk of the acetophenone is strongly adsorbed in the solid phase for the range of temperature of operation.

One can see from Figures 8.14 through 8.16 that the decrease

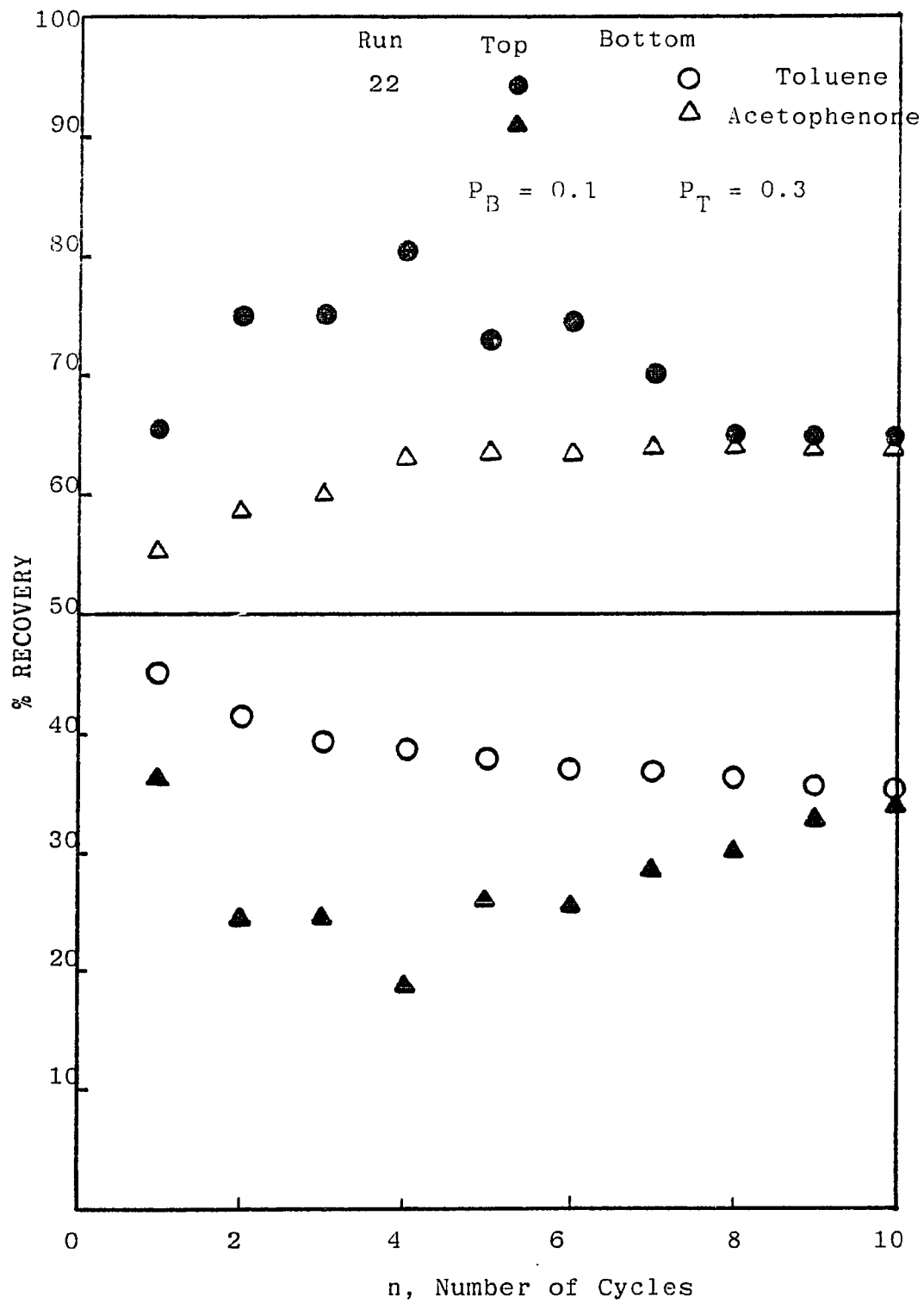


FIGURE 8.16 CONCENTRATION TRANSIENTS FOR $P_T = 0.3$ AND $P_B = 0.1$

of P_T produces an increase in the steady state top product percent recovery of toluene and thus a decrease in the concentration of acetophenone. However, the transient time for the enrichment of toluene (or depletion of acetophenone) is about the same, and the lowest concentration band (depletion of acetophenone) can be calculated from

$$\frac{\langle y_{T2} \rangle_n}{y_0} = \left(\frac{P_T}{1 + P_B} \right)^{2n-2} \quad (4.84)$$

For a given value of P_B by adjustment of P_T to an arbitrarily low value, we may obtain an arbitrarily high degree of depletion of acetophenone in the top product stream. The recovery of toluene in the top product is about 100% in the seventh cycle (Fig. 8.14) for $P_T=0.1$ and $P_B=0.3$; and about 97% in the same cycle (Fig. 8.15) for $P_T=0.2$ and $P_B=0.2$. But for $P_T=0.3$ and $P_B=0.1$, the percent recovery of acetophenone decreased to about 19% on the fourth cycle and took an upward turn thereafter approaching the bottom product concentration. The reason for this phenomena is apparent, since $L_{\text{acetophenone}}(T_1) > L_{\text{acetophenone}}(T_2)$, and $L(T)$ is a function of P_T and P_B , an increase in P_T increases $L_{\text{acetophenone}}(T_1)$ and as a consequence, at T_1 the migration of acetophenone to the inner ends of the column increases for $P_T 0.2$, thereby resulting intermixing of the top and bottom products.

The steady state characteristic solutions for the product concentration for $P_T=0.2$ and $P_T=0.3$ are respectively shown in Figures 8.17 and 8.18. In Figure 8.17, the parapump is operated in such a fashion that all acetophenone characteristics origi-

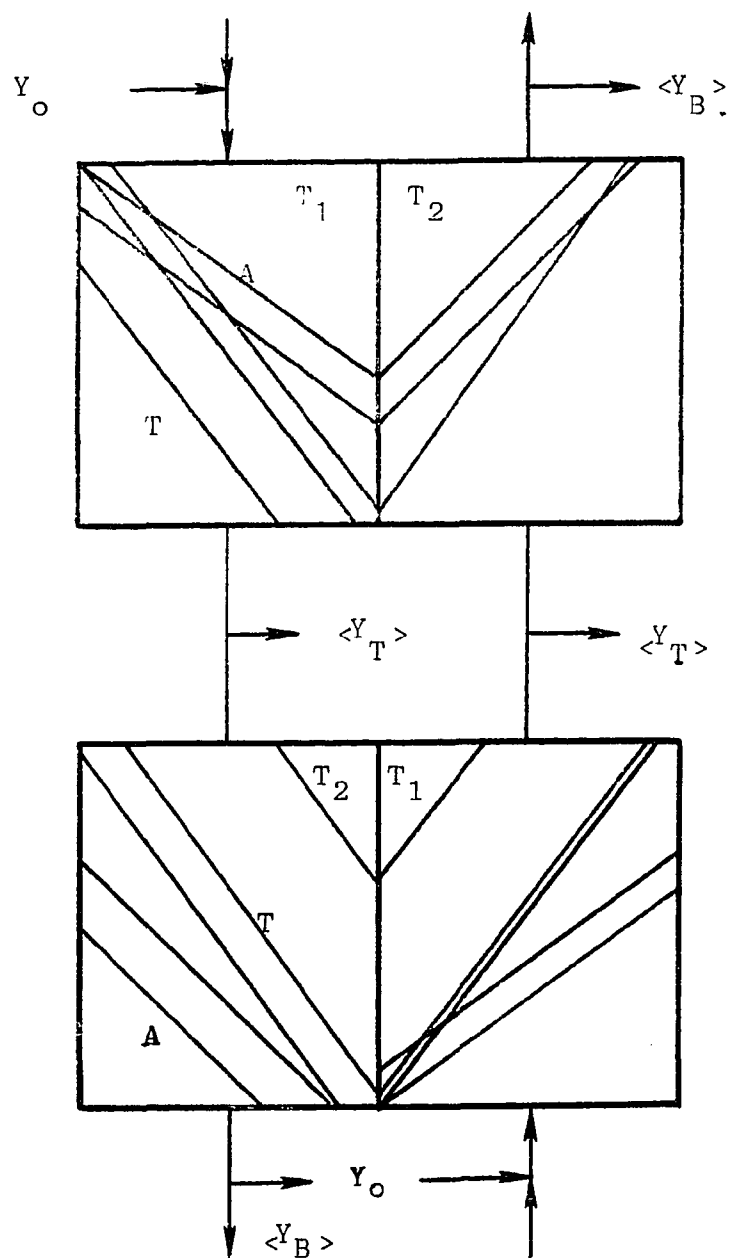


FIGURE 8.17 STEADY STATE CHARACTERISTICS FOR $P_B = P_T = 0.2$

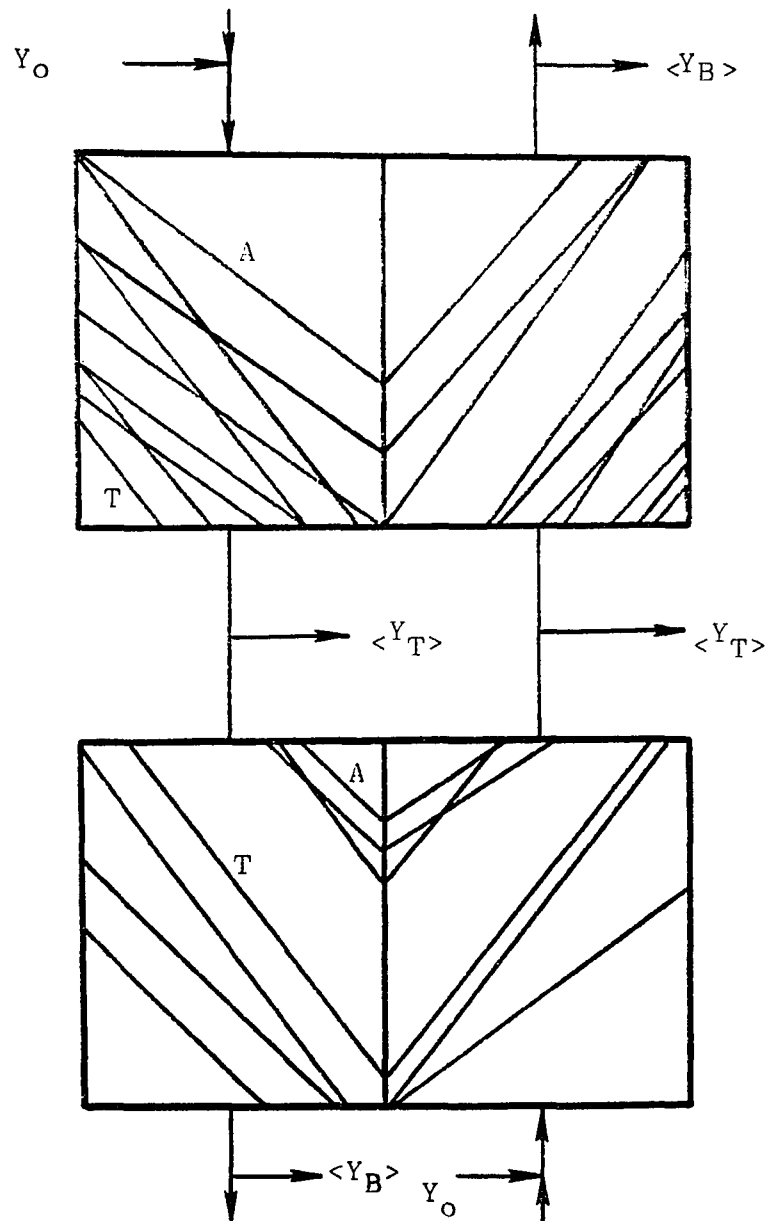


FIGURE 8.18 STEADY STATE CHARACTERISTICS FOR $P_B = 0.1$, $P_T = 0.1$

nating at the outer ends of the column at the point of entry of the feed and solution from the reservoir exit at the top, hence most of the acetophenone entering the column eventually leaves in the bottom product and $\langle y_{T, \text{acetophenone}} \rangle_{\infty} / y_{O} = 0$ for certain values of P_T . In Figure 8.18, the amount of top product, P_T , withdrawn is too much and breakthrough of some of the acetophenone from the bottom product material occurs in the top product and reduces the percent recovery of toluene. Therefore the material which breaks through in the top gradually reduces the recovery, hence $\langle y_T \rangle_n / y_{O} \approx \langle y_B \rangle_n / y_{O}$ (see Fig. 8.16).

Figure 8.19 illustrates a case where the total feed introduced is about half the amount introduced in previous cases. This time $P_B + P_T = 0.2$, but $P_T = 0.1$. The results indicate that the size of the feed has little or no effect on the steady state separation, but the greatest determining factor on the percent recovery is the amount of top product, P_T withdrawn. The acetophenone concentration decreased gradually to essentially 0.00%, while the concentration of toluene increased to about 100% at about the fifth cycle. The concentration of acetophenone in the bottom product also increased gradually and steadied to a value of about 62%, while that of toluene to about 38%. In the runs with $P_B + P_T = 0.4$ (see Figs. 8.14 through 8.16), the steady state value was approached more sharply (at about the third cycle) than with the run where $P_B + P_T = 0.2$ was employed. The latter case ($P_B + P_T = 0.4$) corresponds to a total of 16 cc of feed solution introduced per half cycle. Before the start of the run,

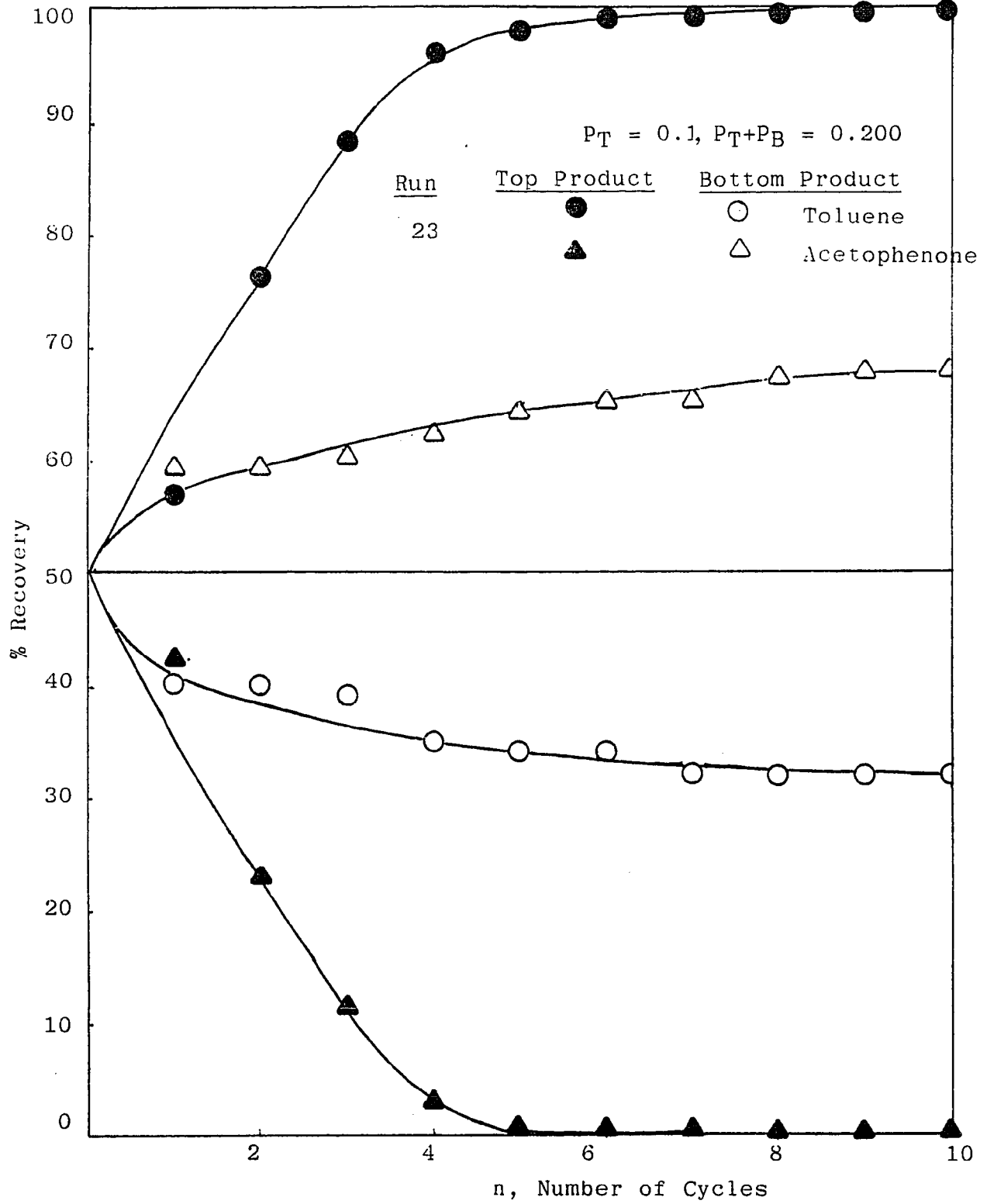


FIGURE 8.19 CONCENTRATION TRANSIENTS FOR $P_T = 0.1$ AND $P_B = 0.1$

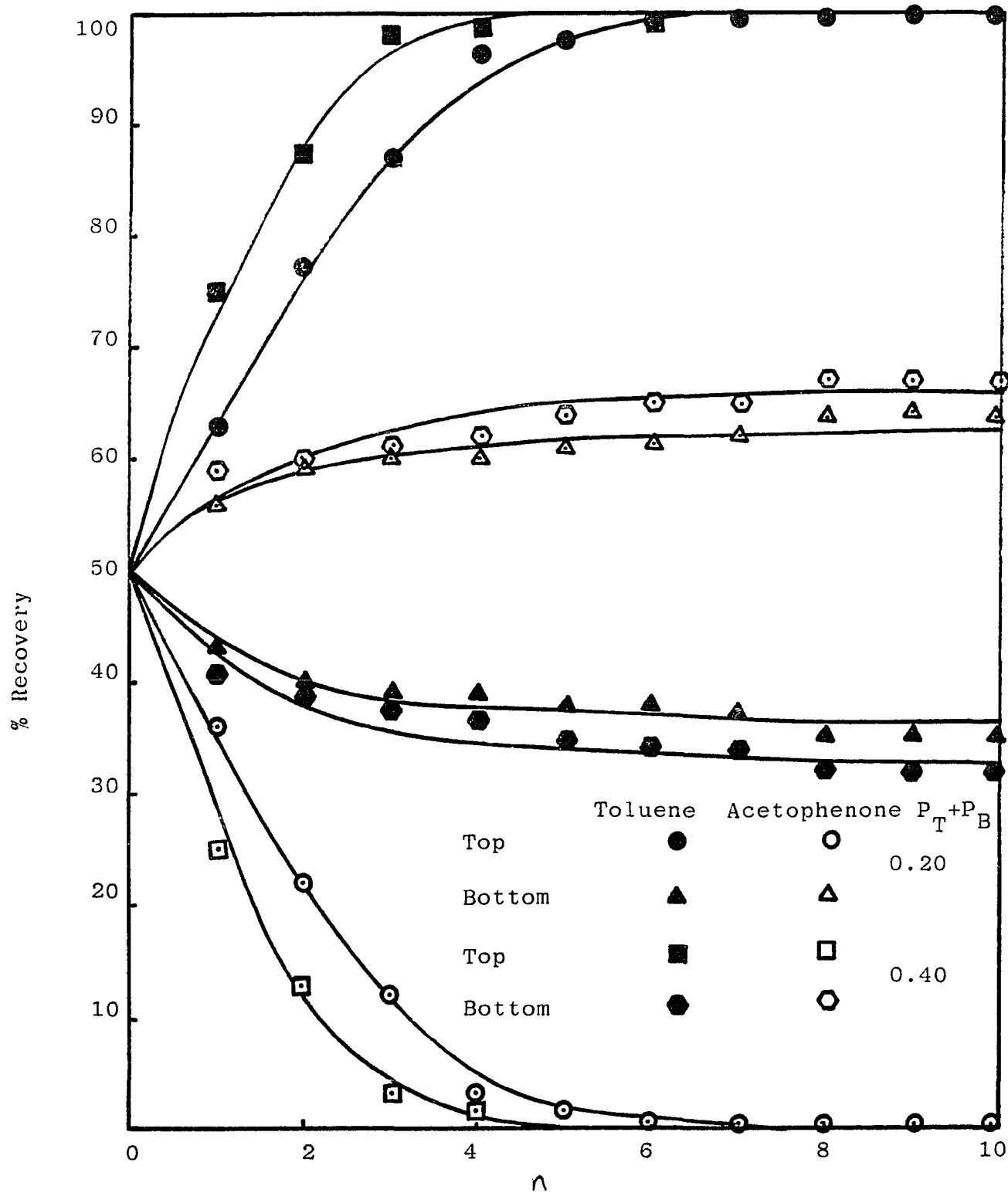


FIGURE 8.20 EFFECT OF FEED RATE ON CONCENTRATION TRANSIENTS

the entire column was saturated with the feed solution. By introducing a feed solution of about 16 cc in every half cycle, more fluid is used to displace the initial concentration of the column, and since the penetration of acetophenone is much less than the penetration of toluene, with proper adjustment of P_T a breakthrough of acetophenone is prevented, but in the case of $P_B+P_T=0.2$, 8 cc of feed solution is introduced, and more cycles are required to displace the initial concentration of the column. Figure 8.20 illustrates a comparison of the two cases. One can see that the steady state concentrations for the two cases are virtually the same.

In Figure 8.21, the effect of top product withdrawal rate on the recovery of toluene (or depletion of acetophenone) is illustrated for values of $P_T=0.1$, 0.2 and 0.3 for fixed value of $P_T+P_B=0.4$. The recovery of toluene ranges from a case where 100% separation is achieved to a case where partial recovery is obtained. For $P_T=0.1$, only 4 cc of product is withdrawn from the top. Since the penetration of the solutes is a function of the interstitial velocity which is, in turn, expressed in terms of P_T and P_B , then it is obvious that an increase in P_T would automatically increase the relative movement of any solute. What this means is that when withdrawing about 4 cc of product from the top, the relative movement of acetophenone is such that acetophenone never breaks through or exits the column via the inner ends. Increasing the top product withdrawal rate to $P_T=0.2$ (8 cc), the column interstitial velocity is increased and thus

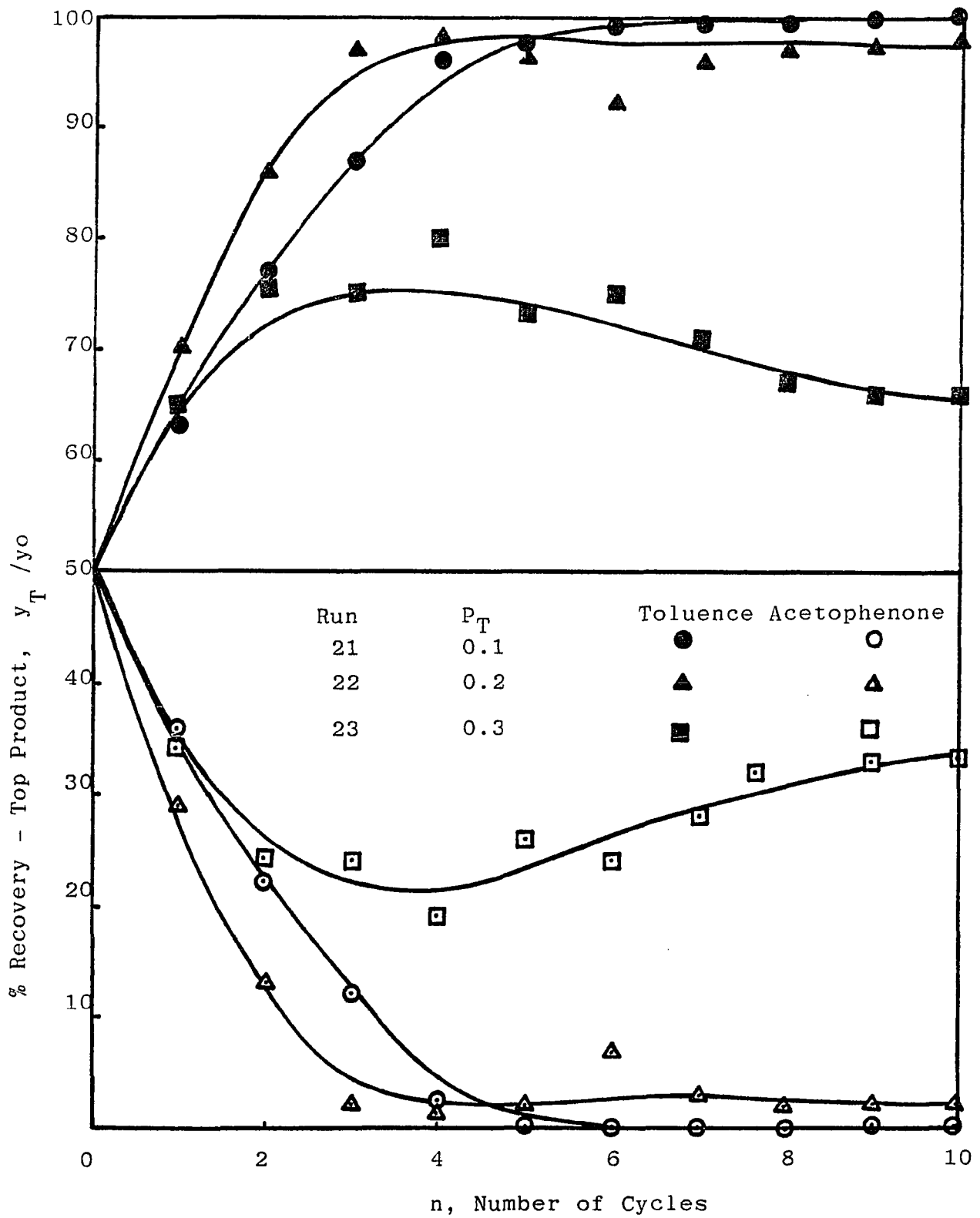


FIGURE 8.21 EFFECT OF TOP PRODUCT WITHDRAWAL RATE ON CONCENTRATION TRANSIENTS

the relative movement of the solutes. By so doing, some of the acetophenone breaks through the column and 98% of toluene is recovered. Based on these results, a trade off can be made in terms of the desired economic viability. A further increase of the top product withdrawal rate to $P_T=0.3$ (12 cc) shows that most of the acetophenone is virtually pumped to the top of the column (inner ends) as the pumping process continues. At steady state the material from the bottom reservoir is pumped to the top product and the two products become equal. This means that if the pump is operated so that $P_T=0.4$ (16 cc) and $P_B=0.0$, there will be no separation and the top product concentration will approach the feed concentration.

The steady state concentration for both toluene and acetophenone as a function of top product withdrawal rate is shown in Figure 8.22. One can see that the steady state concentration of acetophenone in the top product increases from 0.0%, approaching the feed concentration (50%) as P_T increases, while that of toluene decreases from 100% to the feed concentration. The steady state concentration of acetophenone in the bottom product increases from the feed concentration and levels off at about 66%, and that of toluene shows a decrease and levels off at 34%. The dashed lines are extrapolated for $0 \leq P_T < 0.1$. $P_T=0.0$ would correspond to a case where no top product is withdrawn and only product withdrawn from the bottom. For this case, in order to obtain the steady state concentration for the top product, the tubes connecting the two columns together will have to be

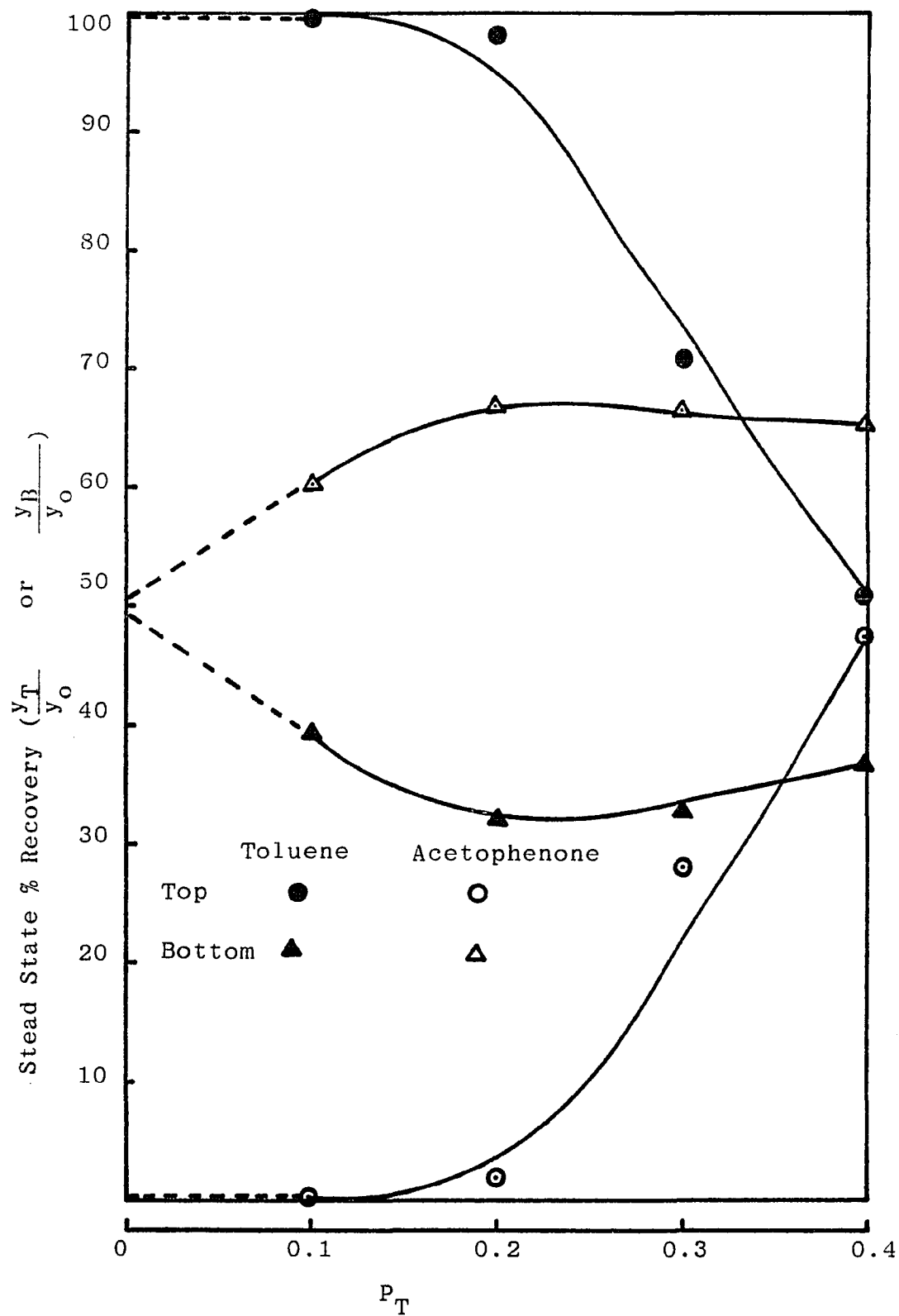


FIGURE 8.22 STEADY STATE CONCENTRATION FOR THE PRODUCTION OF TOLUENE AND ACETOPHENONE IN A TWO COLUMN SYSTEM

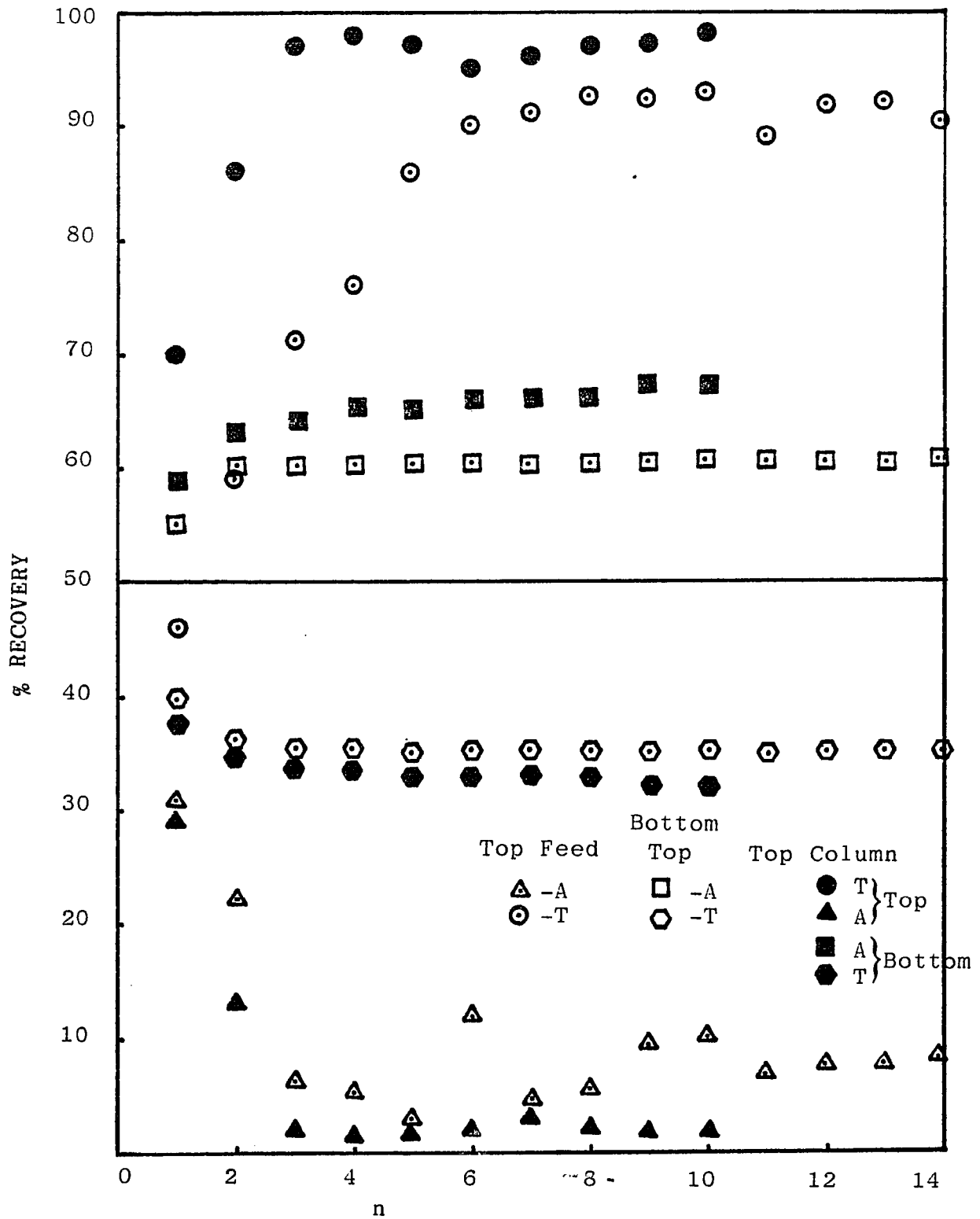


FIGURE 8.23 COMPARISON OF TOP AND BOTTOM FEED CONTINUOUS-ONE COLUMN PARAMETRIC PUMP WITH ALTERNATING TOP AND BOTTOM FEED TWO COLUMN PARAMETRIC PUMPING

carefully disconnected (at the end of the run) in the middle in order to withdraw a sample to determine the concentration. But for $P_T=0.4$, where all of the samples are withdrawn as top product, to determine the steady state concentration for the bottom product, a sample has to be withdrawn from the bottom reservoirs at the end of the entire run.

Figure 8.23 shows a comparison of the recoveries obtained via one column and two column parametric pumping. The data from the one column parametric pumping consist of those from top and bottom feed mode continuous pumps. The data show, in all respects, that two column parametric pumping is superior to the one column, especially for purification of multicomponent systems. The purification of a desired component would, in essence, correspond to the split problem which has received very little attention. Chen et al. (1974), in the analysis of multicomponent separation, claimed that a multicomponent split analogous to that obtained by multicomponent distillation columns could be obtained by proper adjustment of the bottom product withdrawal rate using a single column, but experimental verification was never presented. Butt et al. (1972) also discussed the separation of multicomponent mixtures using a nonsymmetrical flow to force the separation or split with a single column, but experimental treatment was not offered. Gupta and Sweed (1973) presented another theoretical treatment whereby a split could be obtained in a two column configuration using a nonsymmetrical flow pattern. The experimental results of this work may there-

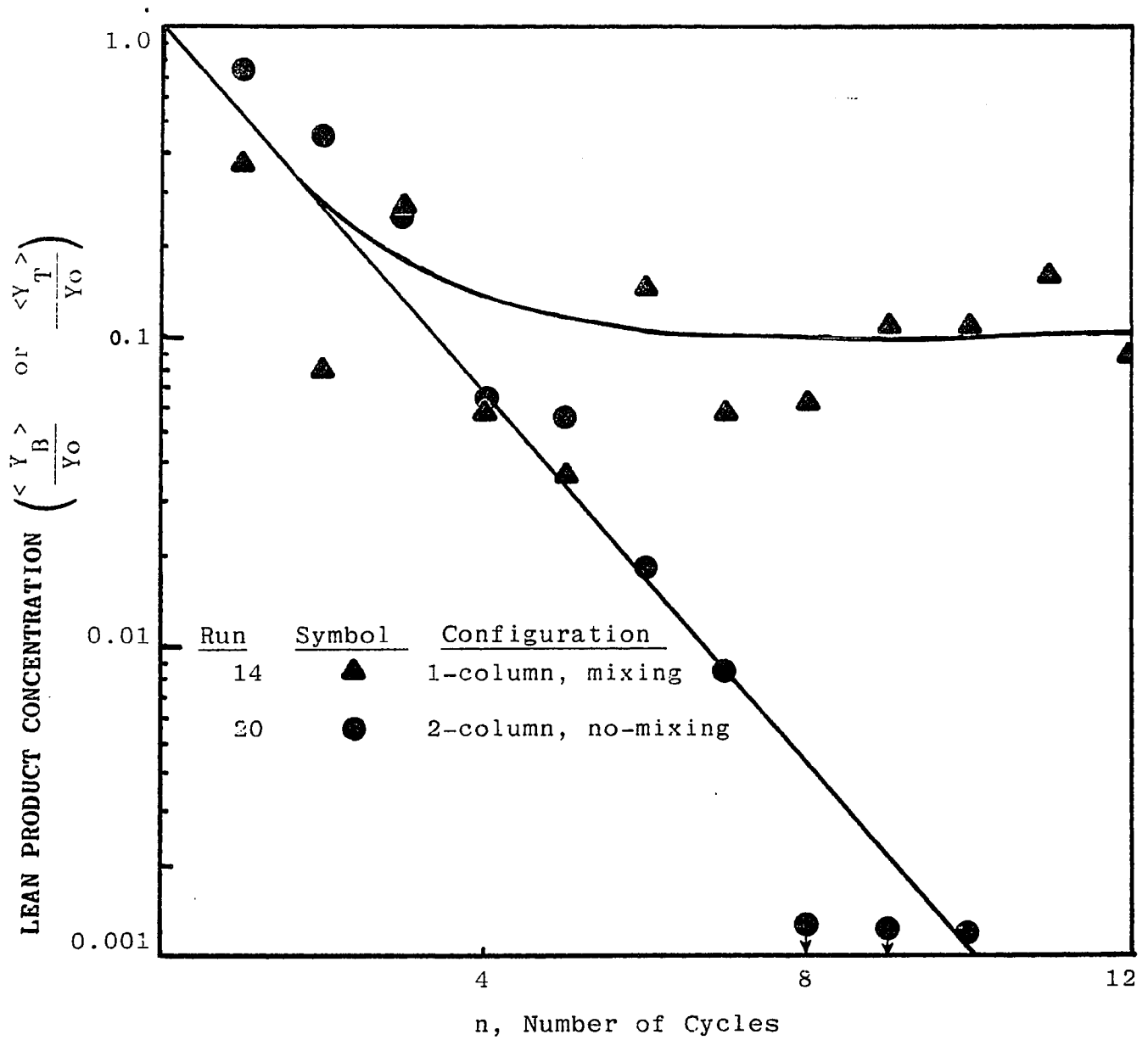


FIG. 8-24 EFFECT OF RESERVOIR MIXING ON PRODUCT CONCENTRATION

fore be considered a breakthrough in achieving a true split with a direct thermal mode parametric pumping using temperature cycling as the only thermodynamic variable.

Figures 8.24 and 8.25 show the effect of reservoir mixing on the separation of multicomponent mixtures. For the mixed reservoirs, data from one column operated semicontinuously are being compared with data retrieved from two column processes with alternating top feed. In both figures, and for the purpose of clarity, a pseudobinary system is assumed where the concentration of acetophenone in the lean product is considered. For the conditions shown the concentration with no mixing are lower than the concentration with mixing. In the results shown, acetophenone concentrations essentially approach zero for the no mixing case, whereas the concentration of acetophenone for the mixing case levels off to values much higher than zero. For operating condition employed, the results of the two column process fits well with the predictions of Chen et al. (1972) that the \log [lean product] versus n , the number of cycles would produce α , where α is the slope obtainable by least squares fit. The relation is true only for parametric pumps operated in the Region 1 regime. In the no mixing case, each element of the fluid leaving one column to the other (inner ends) is not mixed with the elements before it or after it. The only time that mixing occurs is when top product is withdrawn. The top product would essentially consist of fluid elements that have undergone a series of temperature changes between the two columns before

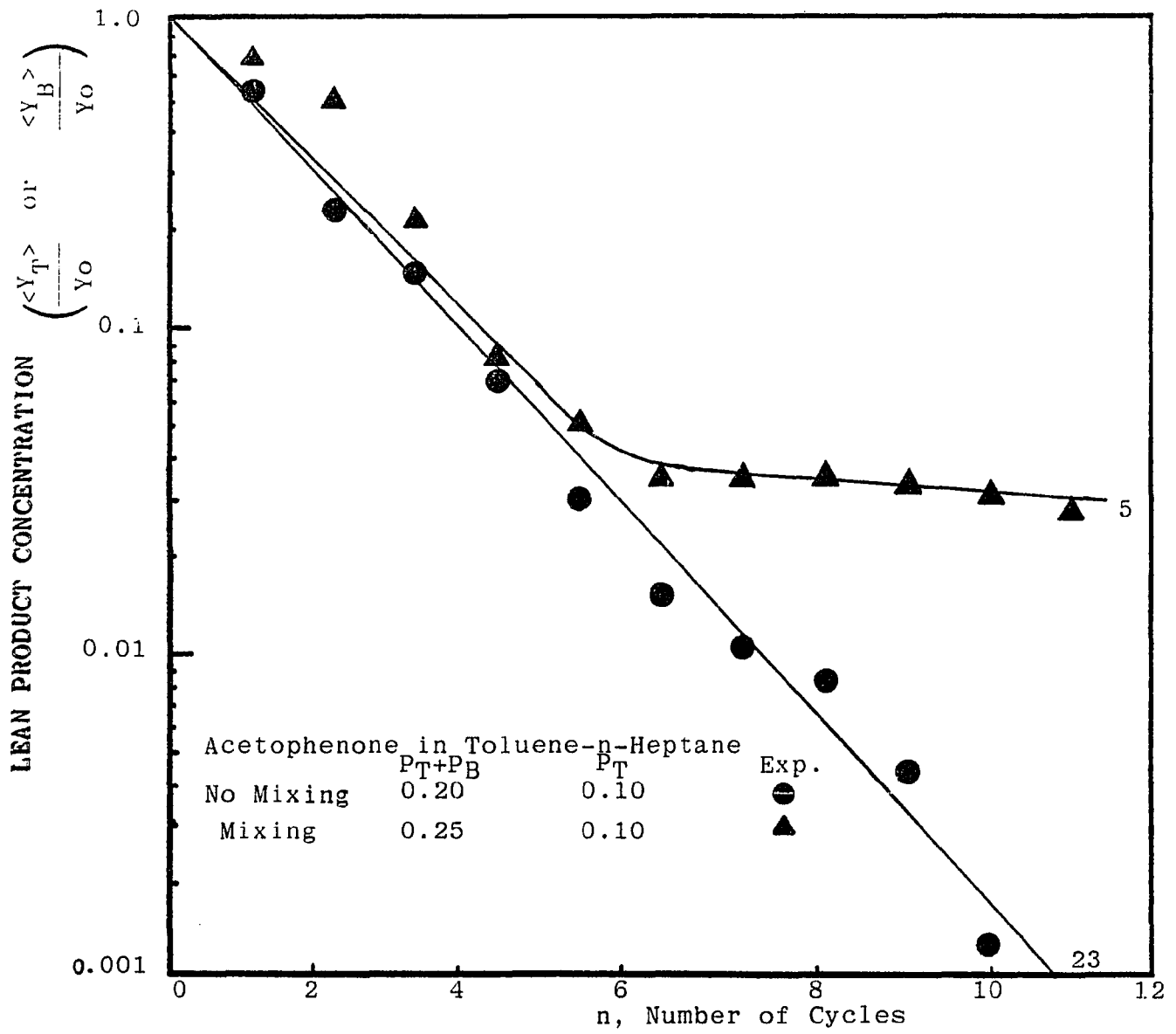


FIGURE 8.25 EFFECT OF MIXING ON MULTICOMPONENT SEPARATION

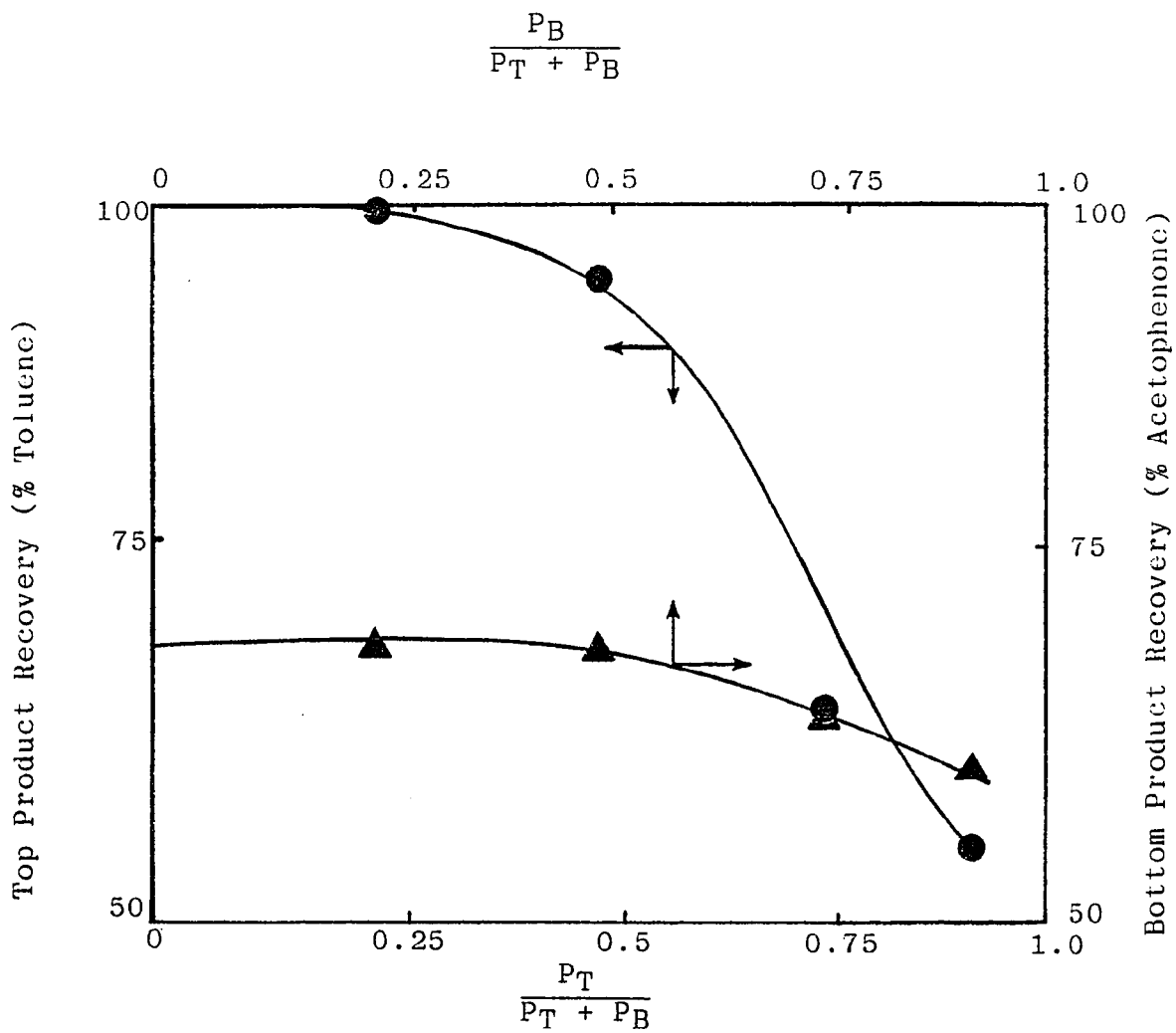


FIGURE 8.26 EFFECT OF PRODUCTION RATE ON SOLUTE CONCENTRATION

they are finally withdrawn as product. Since separability in this case would be measured by the degree of purification of acetophenone, and by the nature of the experimental arrangement, discriminatory withdrawal of desired dilute material can not be made, while the undesired concentrated material is recycled (Wankat, 1978). For the mixed reservoir, each sample product represents a sequential averaging of solute concentration.

Figure 8.26 illustrates a comparison of steady state concentrations for the recovery of toluene and acetophenone. This plot shows the degree of enrichment for both toluene and acetophenone. The enrichment of toluene occurs in the top product, while that of acetophenone occurs in the bottom product. For values of $[P_T/(P_T+P_B)] \leq 0.25$, corresponding to $P_T \leq 0.1$, no acetophenone appears in the top product stream and 100% of toluene is recovered. Beyond $P_T=0.1$ the percentage recovery of toluene decreases with increasing $P_T/(P_T+P_B)$ and will be equal to the feed concentration (50%) when all of the products are withdrawn from the top stream ($P_T=0.4$). The bottom stream (enrichment of acetophenone) is not very sensitive to the size of bottom product. For $[P_B/(P_T+P_B)] \leq 0.60$, the percent recovery of acetophenone is about 67% and for $0.60 < [P_B/(P_T+P_B)] \leq 1.0$, the percent recovery shows only a slight drop from 67% to about 53%.

ONE COLUMN STAGED SEQUENCE CYCLIC PROCESS

Figure 8.27 through 8.34 show the experimental results obtained from one column cycling zone adsorption/desorption process. The results are cyclic steady states where each cycle

is a repeat of the cycle before it. This limiting condition where a cyclic steady state is obtained has been theoretically proven by Wankat (1973), and Lavie and Rielly (1972). The aim of these cycling zone experiments is to establish the necessary conditions for the design of a staged sequence cyclic process.

Thermal wave velocity, u_{th} has been shown by wankat (1973) to be insensitive to temperature, but that if series of temperature step inputs are imposed as the cyclic variable, the size of the step inputs will determine the thermal wave velocity. In the original work on cycling zone, Baker and Pigford (1971) defined the travelling wave (recuperative) and standing wave (direct) mode of cyclic operation. The latter being the case where the fluid is heated/cooled before it is pumped through the adsorbent column, while in the later case, the column walls are heated/cooled directly during the course of operation. The thermal velocity of the travelling wave can be made to approach that of the standing wave if the natural thermal velocity can in fact be made to approach infinity ($u_{th} \rightarrow \infty$). However, for a cycling zone process operating at high frequency (short thermal switching period), the ideal direct thermal mode (where $u_{th} \rightarrow \infty$) can never be obtained because the column temperature is always changed before the original column temperature reaches steady state. Therefore the mode of operation of the cycling zone experiments done in this study could neither be classified as a recuperative nor direct mode. The physical operation itself is direct mode, but the response of the temperature imposed on the column is not instantaneous (normally assumed by most research-

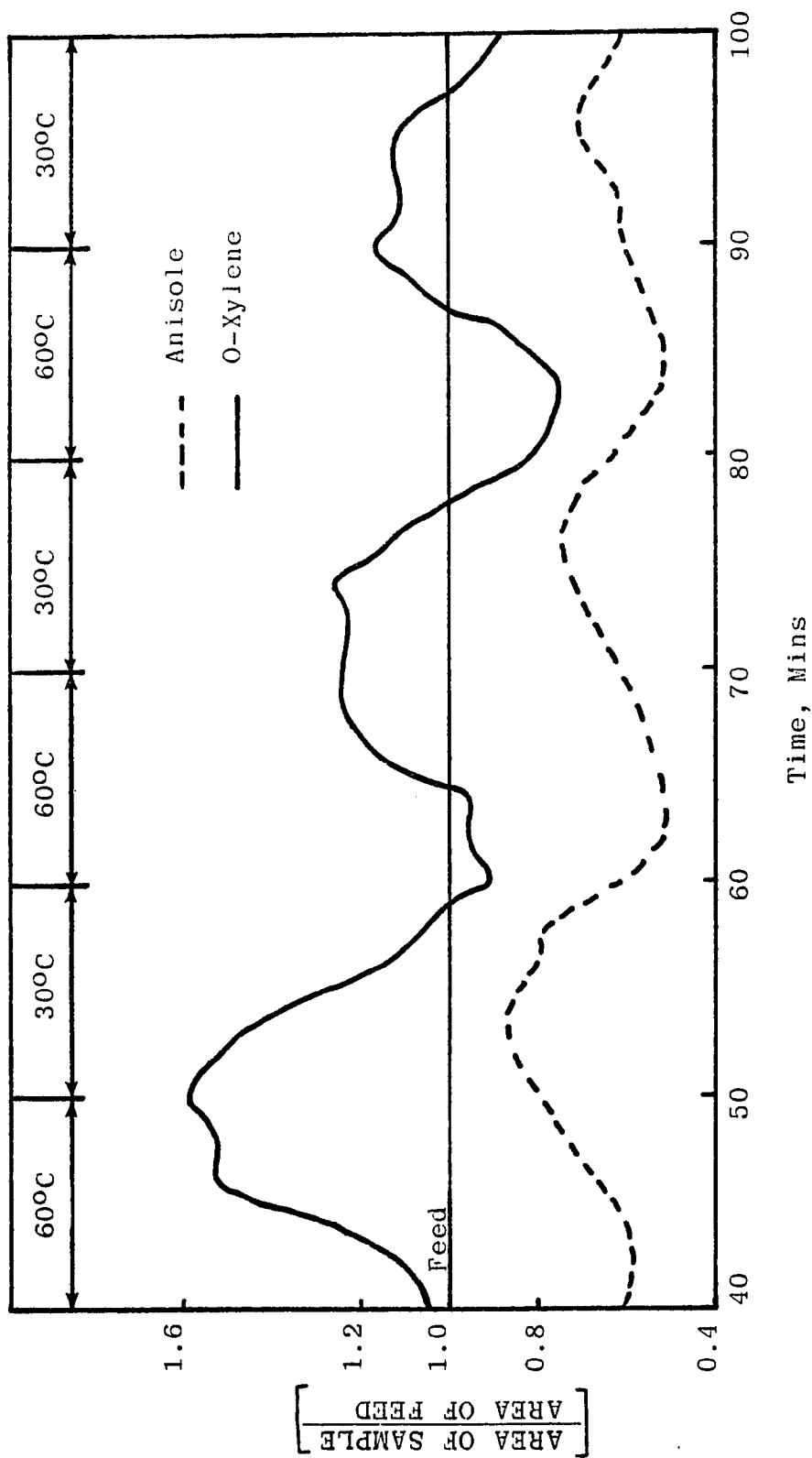


FIGURE 8.27 CONCENTRATION OF O-XYLENE AND ANISOLE AT LOWER TEMPERATURE LEVEL. THERMAL SWITCHING PERIOD: $t_{30}=t_{60}=10$ mins, $L_{th}>L_{o-xylene(60)}>L_{Anisole(60)}$; $L_{th}>L_{o-xylene(30)}>L_{Anisole(30)}$

ers) which is characteristic of direct mode of operation.

Wankat (1974) defined a parameter A , which is a function of the heat capacities of the mobile and solid phases and the column material, that is analogous to Baker and Pigford's (1971) u_{th} . The shape of u_{th} is a square wave and it is greater than u_c (concentration wave velocity) if $A = 1.0$. When $A = 1.0$, a square temperature wave is attained, meaning that the moment the column temperature is changed, an instantaneous response of the exact temperature is attained. Instantaneous temperature change does not necessarily mean maximum separation. The effect of A on the separation has been theoretically investigated by Wankat (1974) and found that there exists an optimum value, where $0.0 < A < 1.0$ for which maximum separation can be obtained. Therefore all the experimental strategies in this study and hence the values of A are based not on the adjustment of the heat capacities of the system materials but on the temperature cycling frequency (Wankat, 1973). Based on the same line of reasoning, the temperature wave can be expressed in terms of the penetration distances (Chen and Hill, 1971a) where L_{th} is the penetration distance of the thermal wave and $L_i(T)$ is the penetration distance of component i at temperature T .

Various characteristic concentration profiles have been observed based on the adjustment of L_{th} . By proper adjustment of L_{th} , the amplification of solute concentration (Baker and Pigford, 1971) could be obtained. Figure 8.27 shows the effluent concentration versus time for the system *o*-xylene-anisole-*n*-heptane on silica gel.

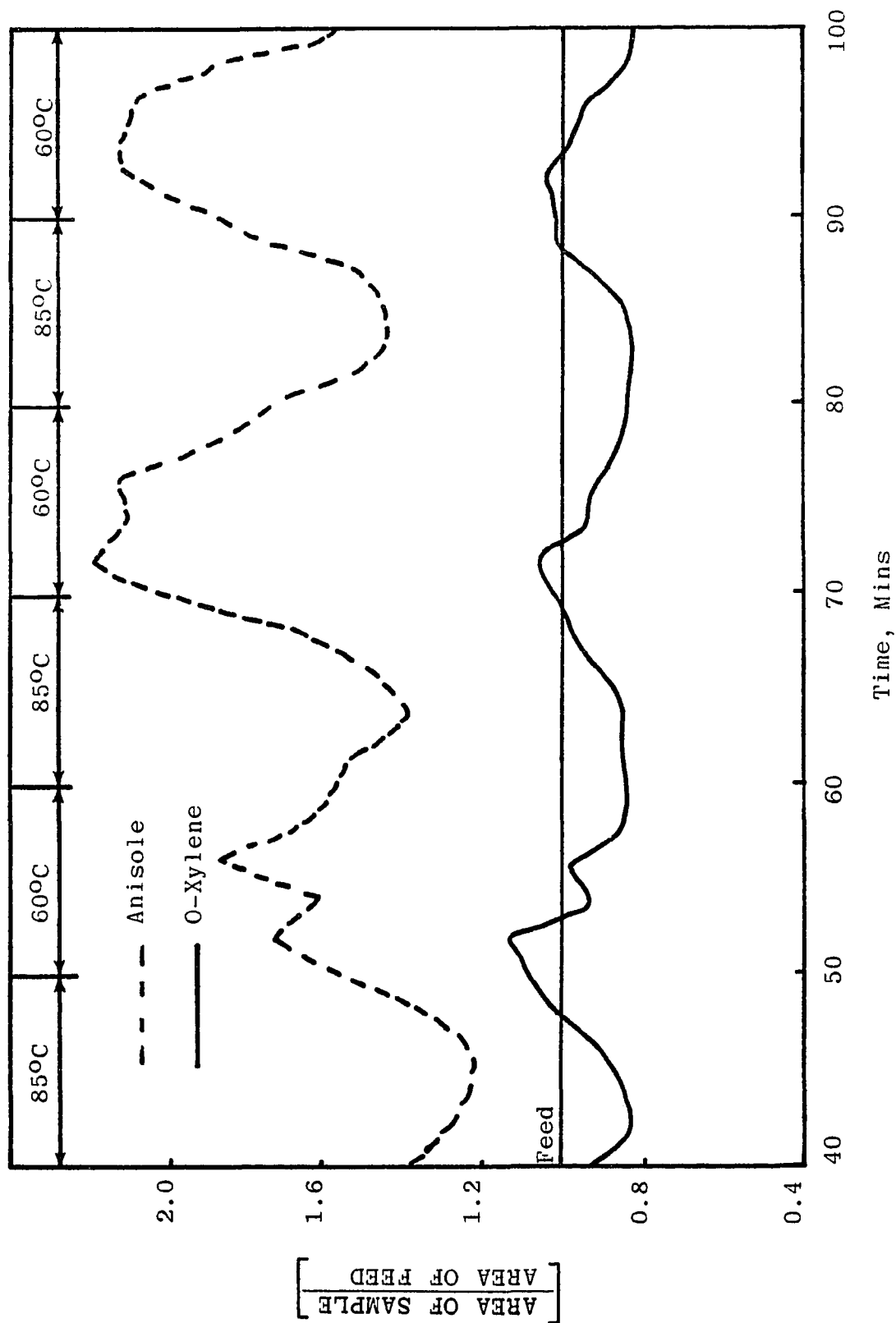


FIGURE 8.28 CONCENTRATION OF O-XYLENE AND ANISOLE AT UPPER TEMPERATURE LEVEL
 THERMAL SWITCHING PERIOD:
 $t_{60}=t_{85}=10$ mins, $L_{th}>L_{Anisole}(85)>L_{o-xylene}(85)$; $L_{th}>L_{Anisole}(60)$
 $L_{o-xylene}(60)$

This run was performed in the lower temperature level, viz: $T_1(=30^\circ\text{C})$ and $T_2(=60^\circ\text{C})$. These temperatures are chosen so that o-xylene can be concentrated between the thermal boundary T_1 and T_2 while anisole will not. The cyclic behavior of the concentration profile with change in temperature can easily be seen. At 30°C , o-xylene and anisole are adsorbed and their concentrations even at 30°C would eventually approach the feed concentrations. So for all runs, the frequencies of thermal switching periods are chosen so that these limiting concentrations at low frequencies are prevented. At 60°C , the concentration of o-xylene increases somewhat but still below the feed level. For this run the thermal switching period is $t_{30}=t_{60}=10\text{mins}$, and under this operating condition, $L_{th} > L_{o\text{-xylene}(60)} > L_{\text{anisole}(60)}$ and $L_{th} > L_{o\text{-xylene}(30)} \approx L_{\text{anisole}(30)}$.

The condition where $u_{th} > u_h > u_c$ (u_h =concentration during hot cycle and u_c = concentration during cold cycle) (Wankat, 1978), and thus $L_{th} > L_i(T_2) > L_i(T_1)$ are typical of most liquid systems. One can also see that the concentrations of both solutes lag behind L_{th} since the solutes peak exact on the thermal boundary.

Figure 8.28 illustrates a case where the cycling zone is operated at the higher temperature level i.e., at $T_2(=60^\circ\text{C})$ and $T_3(=85^\circ\text{C})$. The thermal switching period is $t_{60}=t_{85}=10\text{ mins}$. One obvious behavior noticeable from this figure is that it appears as if the maximum peaks for both o-xylene and anisole occur at 60°C . In reality the solutes peaked at 85°C but there is a tremendous concentration lag behind the thermal velocity. This

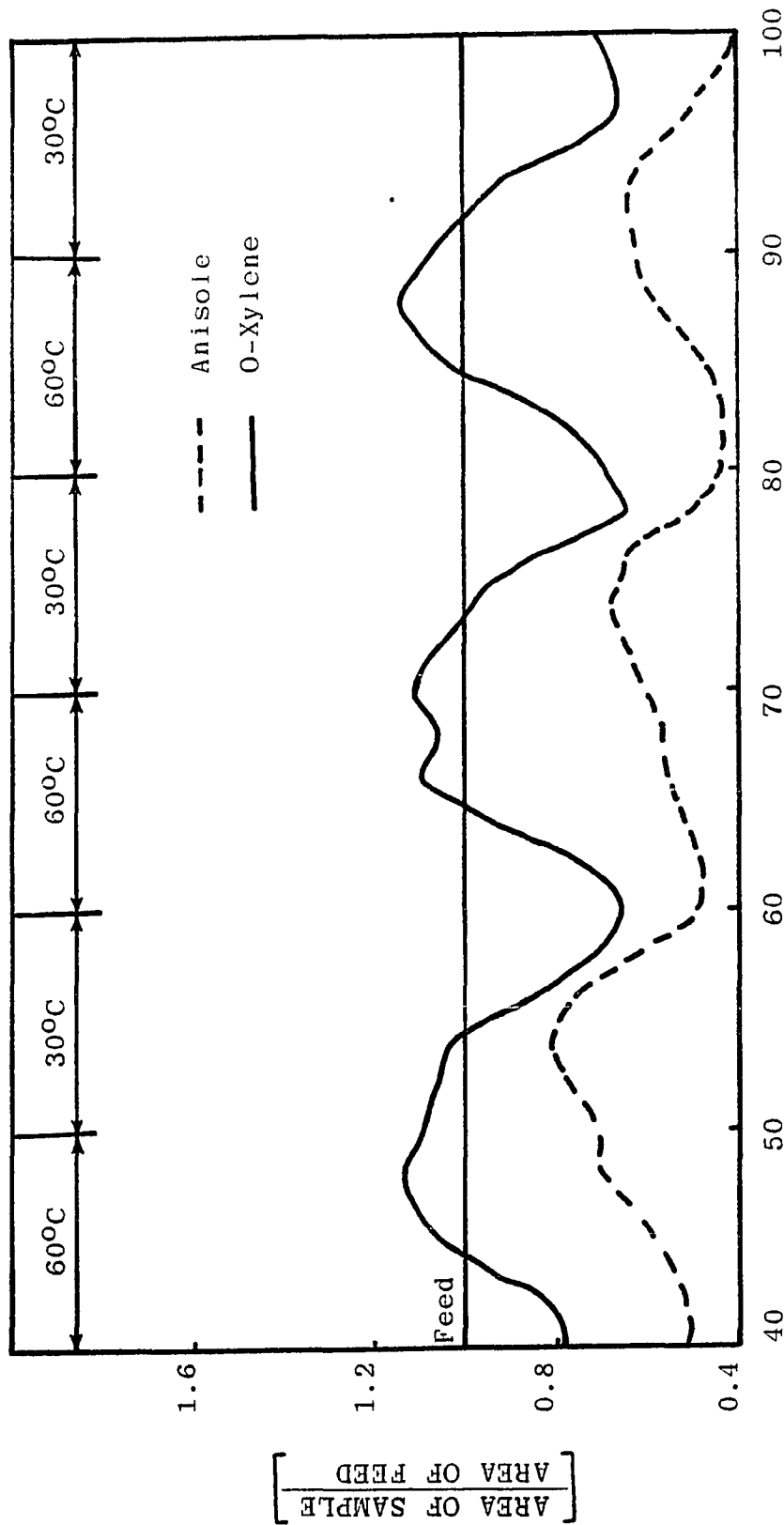


FIGURE 8.29 CONCENTRATION OF O-XYLENE AND ANISOLE AT LOWER TEMPERATURE LEVEL
 THERMAL SWITCHING PERIOD:
 $t_{30=t_{60}=10 \text{ mins}}$, $L_{o\text{-xylene}(60)} > L_{th} > L_{o\text{-xylene}(30)}$; $L_{th} > L_{\text{Anisole}(60)} > L_{\text{Anisole}(30)}$

is to say that $L_{th} > L_{anisole(85)} > L_{o-xylene(85)}$ and $L_{th} > L_{anisole(60)} > L_{o-xylene(60)}$. Also at this temperature level, the concentration of o-xylene is around the feed level at both temperatures, the reason for this is that the cyclic process is not operated in a temperature range to allow for enough o-xylene to be adsorbed and therefore subsequently desorbed. In effect o-xylene and heptane both act as solvent at this temperature range. Figure 8.29 shows where the cyclic process is again operated at the lower temperature level. All the operating variables are the same as that shown in Figure 8.27 except that it is operated in a fashion such that $L_{o-xylene(60)} > L_{th} > L_{o-xylene(30)}$ and $L_{th} > L_{anisole(60)} > L_{anisole(30)}$. To be able to over ride the natural thermal penetration distance it would require a special artistry when the cyclic process is being operated. Initially when the temperature is switched from 30°C to 60°C, the thermal wave moves behind the concentration wave, and during the course of operation the thermal wave gradually over takes the concentration wave. If the thermal wave is allowed to maintain this speed till the end of t_{60} , o-xylene will peak at the temperature boundary. In order for the o-xylene to peak between T_1 and T_2 , the thermal wave must be slowed down by switching the temperature to the next temperature step so that it does not overtake the concentration wave. The thermal velocities for all the other runs are adjusted by switching the column temperature to the next temperature step about 4 mins before the end of that temperature cycle.

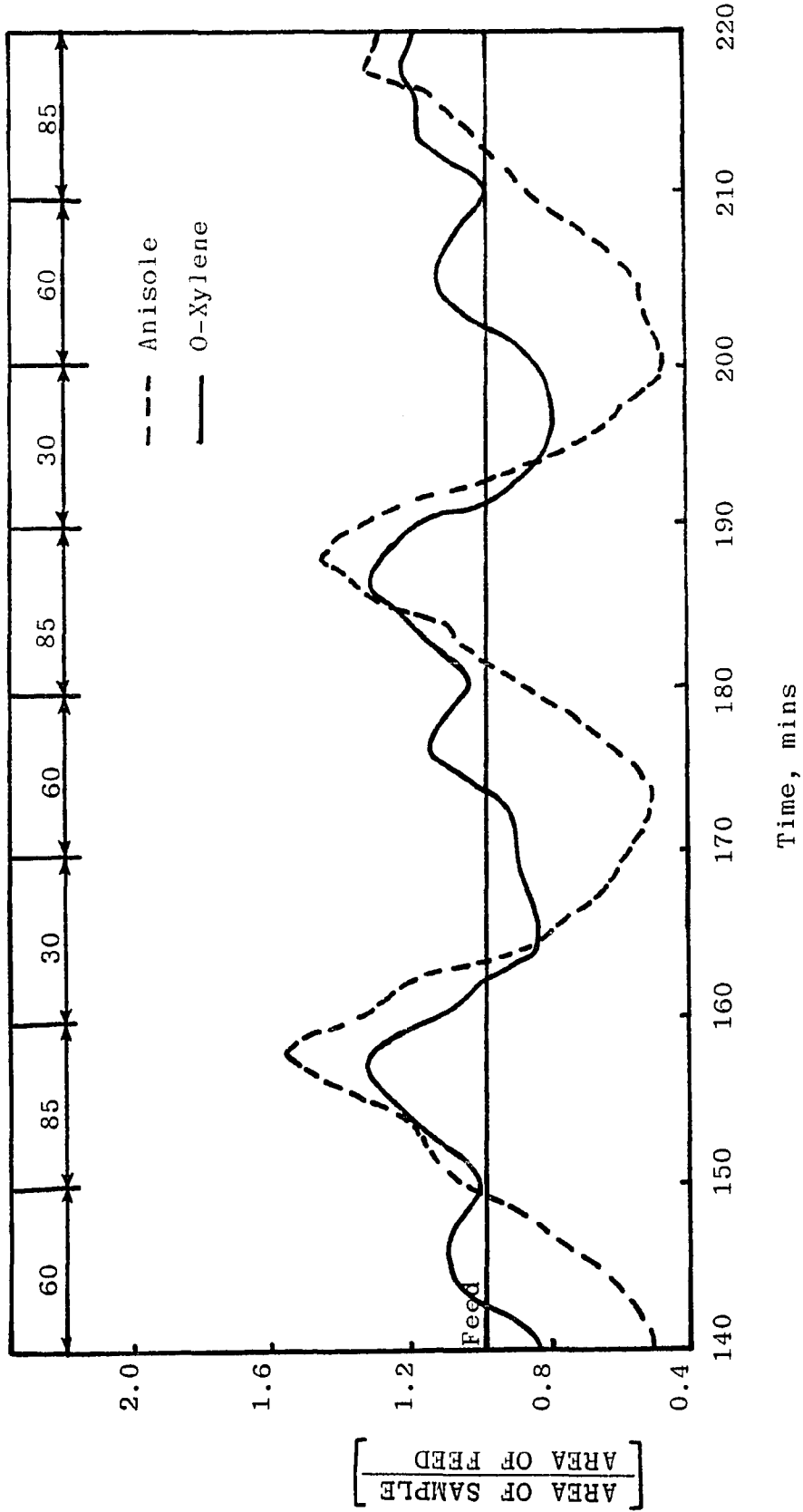


FIGURE 8.30 CONCENTRATION OF O-XYLENE AND ANISOLE AT LOW AND HIGH TEMPERATURE LEVELS
 THERMAL SWITCHING PERIOD: $t_{30=t_{60=t_{85}}=10}$ mins, $L_{o\text{-xylene}(60)} > L_{th} > L_{o\text{-xylene}(30)}$;
 $L_{\text{Anisole}(85)} > L_{th} > L_{\text{Anisole}(60)}$; $L_{o\text{-xylene}(85)} > L_{\text{Anisole}(85)} > L_{o\text{-xylene}(30)}$

In Figure 8.30, the three temperature step inputs were used in operating the cycling zone. For this run, the thermal switching period is $t_{30}=t_{60}=t_{85}=10$ mins. Anisole peaked at 85°C and exhibited a single peak but o-xylene showed double peaks, one at 60°C and the other at 85°C . The reason for this is obvious, at the end of 60°C temperature step, all of the o-xylene did not exit the column completely, and as soon as the column temperature is raised to 85°C , anisole must now exit the column and by so doing it exit the column with the rest of o-xylene, hence the overlap of the second o-xylene peak with anisole. Figure 8.31 also shows the same characteristic phenomena for a cyclic process operated at $t_{30}=t_{60}=t_{85}=14$ mins. The second o-xylene peak does not overlap the anisole peak as much as the case when it is operated at $t_{30}=t_{60}=t_{85}=10$ mins. The reason for this is that more time is allowed for the o-xylene peak to exit the column when it is operated at $t_{30}=t_{60}=t_{85}=14$ mins. However, Figure 8.30 and 8.31 do have one thing in common. The concentration of o-xylene exhibited a dip before the second peak that overlapped the anisole peak. From Figures 8.30 and 8.31, the characteristic behavior of the o-xylene and anisole before or after the dip is inconsistent for any conclusion to be drawn.

In Figure 8.32, the thermal switching periods are $t_{30}=10$ mins, $t_{60}=t_{85}=14$ mins. At 60° and 85°C , o-xylene peak do not show any appreciable increase above the feed concentration. The amount of o-xylene adsorbed at 30°C for $t_{30}=10$ mins are completely desorbed during the 60° and 85°C interval, since the total time for the desorption is about 28 mins. In the case of

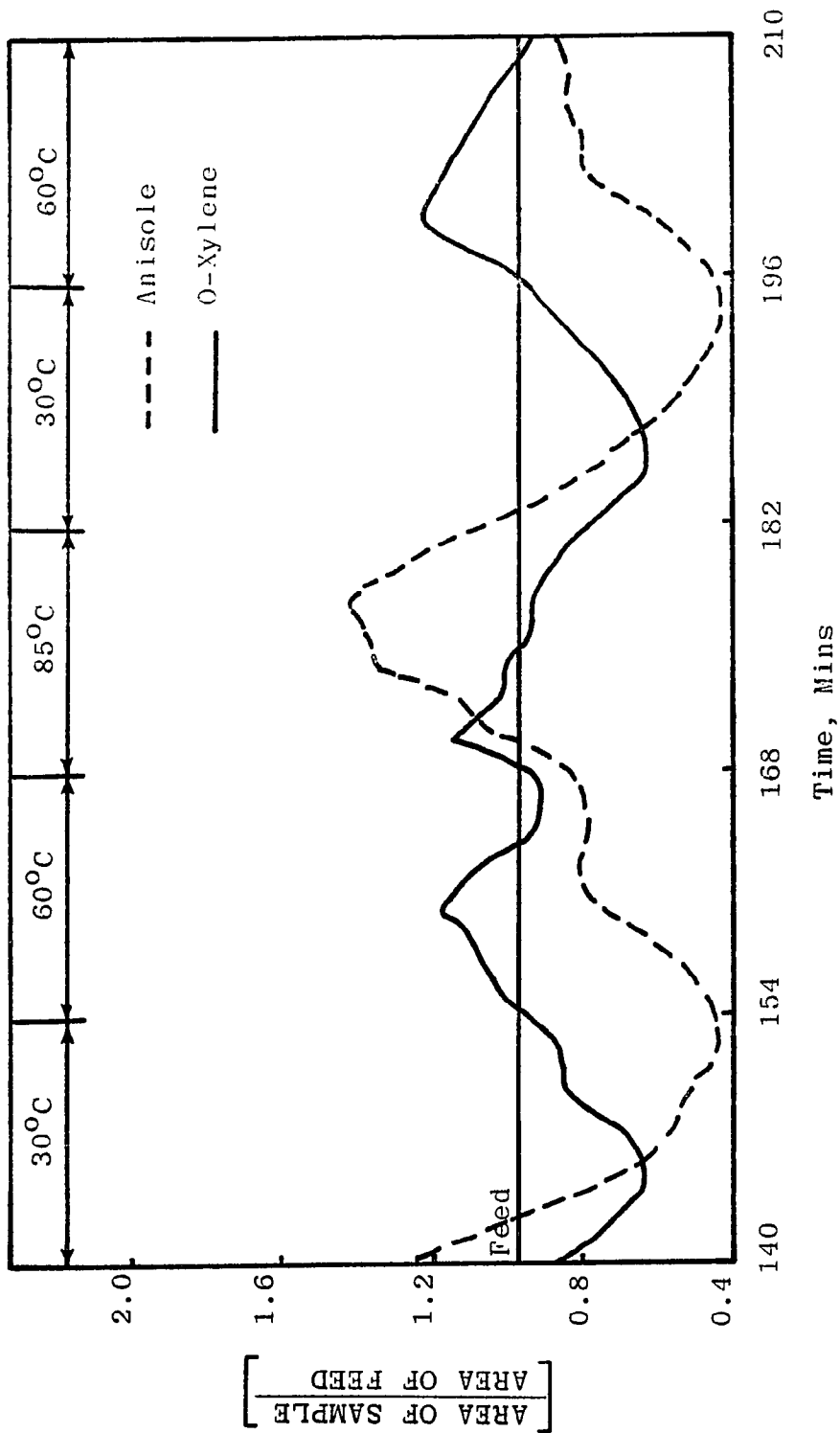


FIGURE 8.31 CONCENTRATION OF O-XYLENE AND ANISOLE AT LOW AND HIGH TEMPERATURE LEVEL
 THERMAL SWITCHING PERIOD: $t_{30} = t_{60} = t_{85} = 1.4$ mins; $L_{O-xylene(60)} > L_{th} > L_{O-xylene(30)}$,
 $L_{Anisole(85)} > L_{th} > L_{Anisole(60)}$, $L_{O-xylene(85)} > L_{O-xylene(30)} > L_{Anisole(30)}$

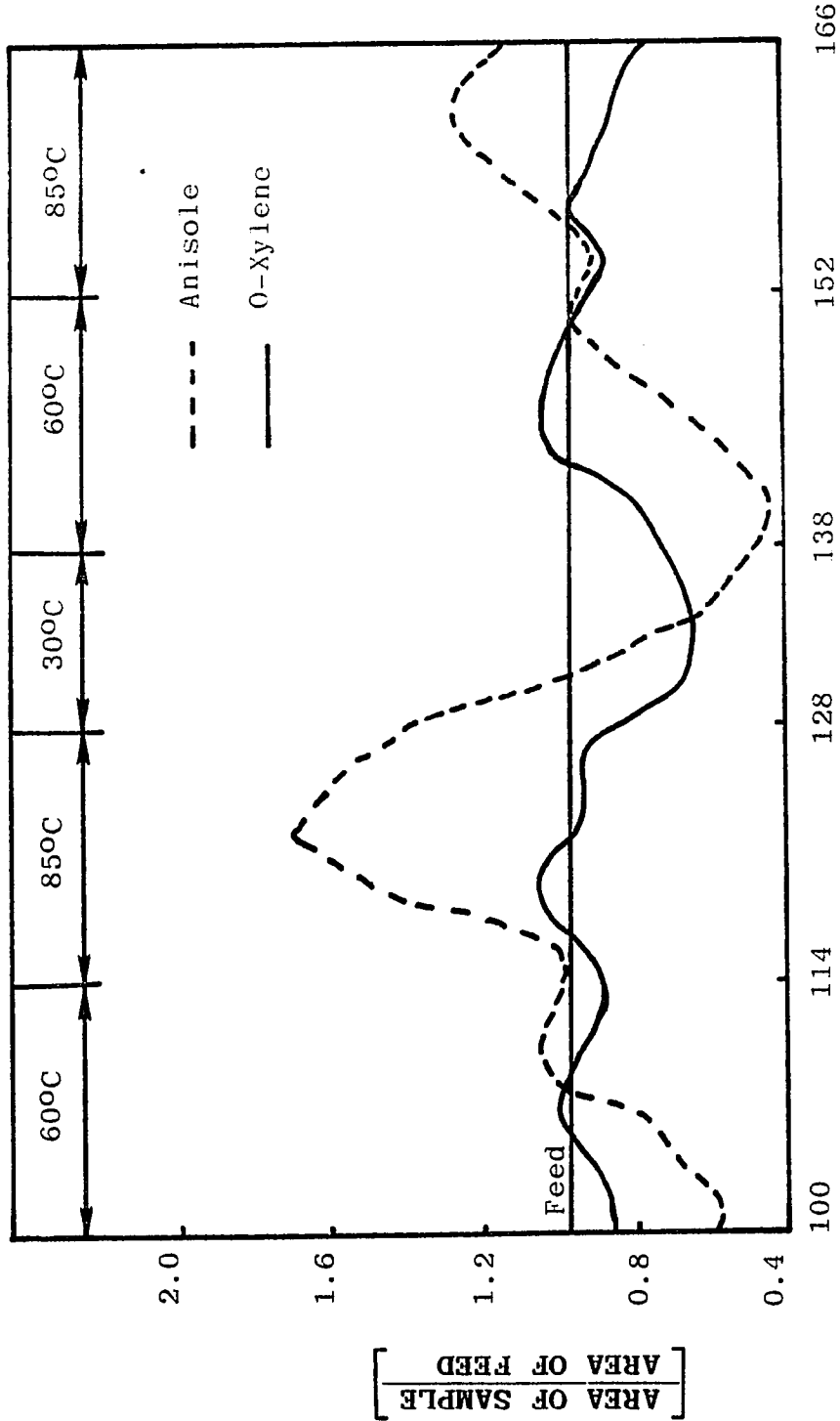


FIGURE 8.32 CONCENTRATION OF O-XYLENE AND ANISOLE AT LOW AND HIGH TEMPERATURE
THERMAL SWITCHING PERIOD: $t_{30} = 10$ mins, $t_{60} = t_{85} = 14$ mins;
 $L_{o\text{-xylene}(60)} > L_{th} > L_{o\text{-xylene}(30)}$, $L_{Anisole(85)} > L_{th} > L_{Anisole(60)}$,
 $L_{o\text{-xylene}(85)} > L_{Anisole(85)} > L_{o\text{-xylene}(30)} > L_{Anisole(30)}$

anisole, about 24 mins of adsorption time is available for anisole to be adsorbed in the column, i.e., $t_{30}=10$ mins and $t_{60}=14$ mins, therefore at the 85°C interval, a much sharper anisole peak is obtained. Increasing t_{30} to 20 mins. (see Figure 8.33) shows almost the reverse of the result obtained in Figure 8.32. A case where the anisole never peaked above the feed concentration can be seen. At the 30° interval which is for a duration of 20 mins, anisole is almost completely adsorbed and it is virtually blocking all the adsorption sites. Since adsorption between the two solutes is competitive, the sites occupied by one solute is almost if not completely void of the other solute. When the temperature is subsequently raised to 60° and 85°C , the concentration of anisole takes an upward trend which is a sign of desorption, but the column is not maintained at this temperatures long enough for the anisole peak to emerge to above the feed concentration. On the other hand, the o-xylene peak fluctuates slightly above and below the feed concentration. In some cases at the 30° interval, the concentration of o-xylene is about the same concentration as the feed, meaning that all the adsorption sites are completely occupied by anisole and as a result, o-xylene is no longer retained in the column.

Figure 8.34 illustrates a situation whereby high solute concentrations could be recovered, while the low concentration regions are recycled. Once all the operating conditions are established, the problem is now reduced to collecting the samples of the desired products manually or automatically knowing the relative retention time of each peak. Continuous

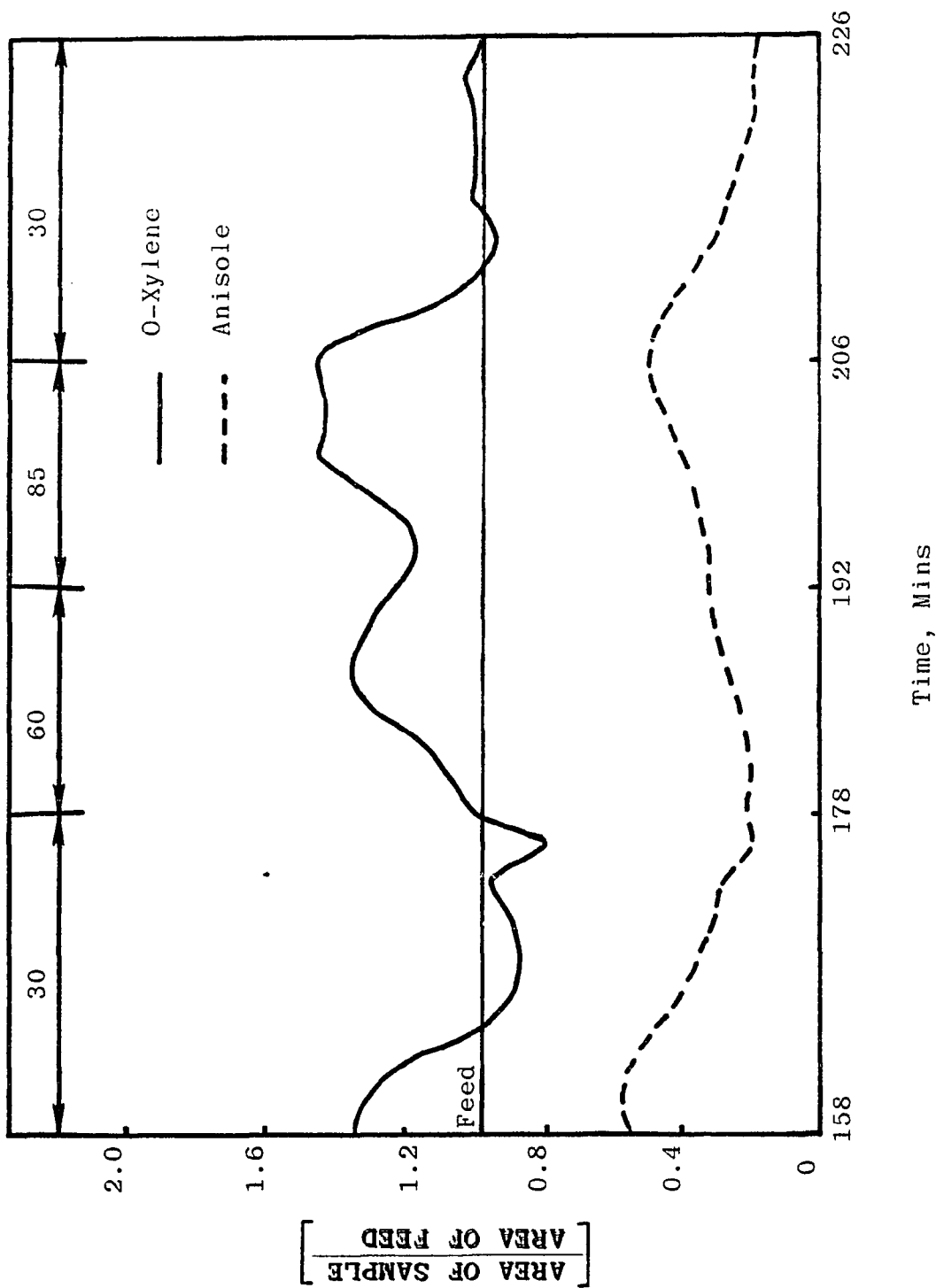


FIGURE 8.33 CONCENTRATION OF O-XYLENE AND ANISOLE AT LOW AND HIGH TEMPERATURE LEVELS
 THERMAL SWITCHING PERIOD: $t_{30} = 20$ mins. $t_{60} = t_{85} = 14$ mins;
 $L_{o-xylene(85)} \approx L_{o-xylene(60)} > L_{th} > L_{o-xylene(30)}$;
 $L_{th} \approx L_{anisole(85)} > L_{anisole(30)} > L_{anisole(60)}$

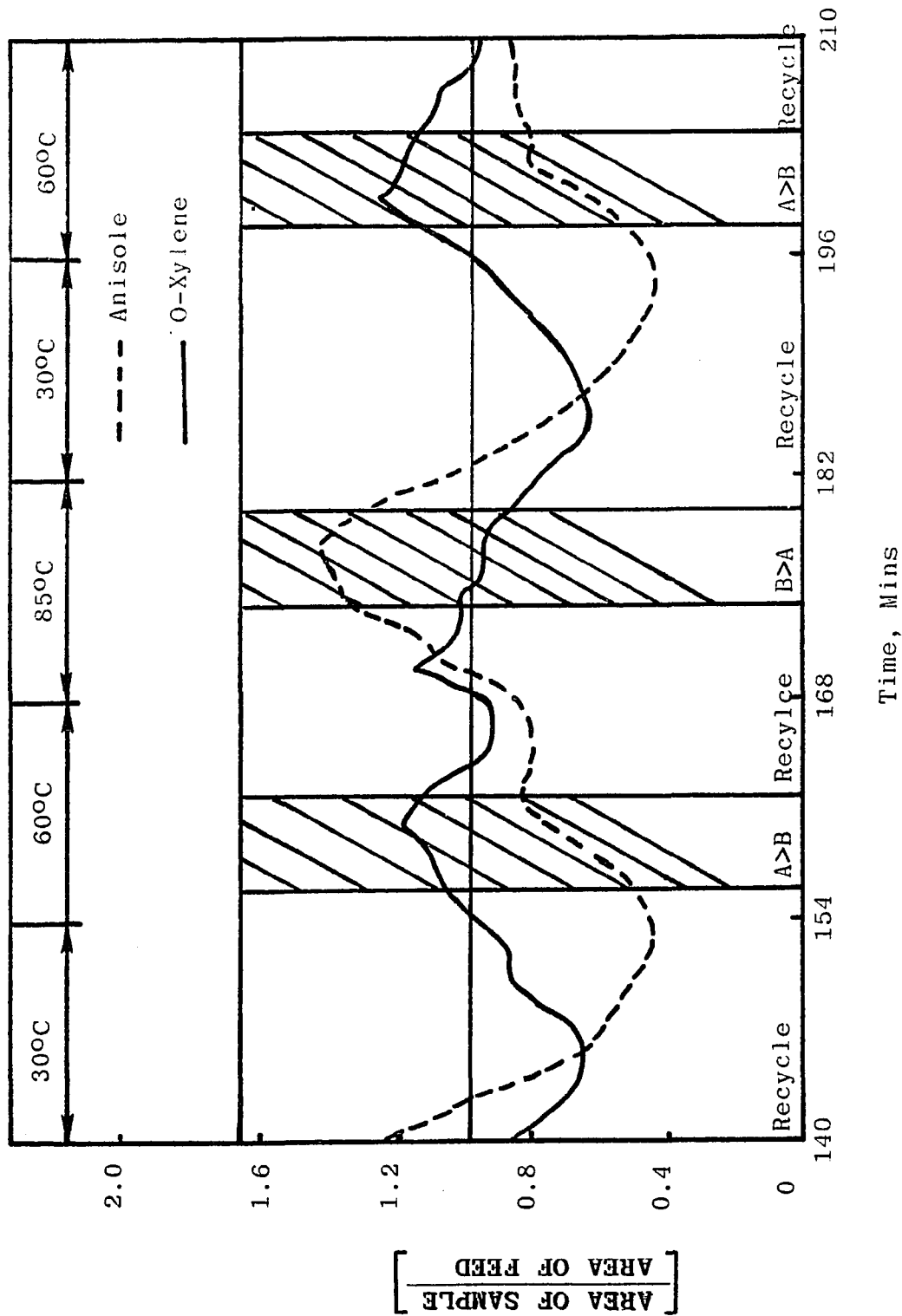


FIGURE 8.34 RECOVERY OF O-XYLENE AND ANISOLE THERMAL SWITCHING PERIOD:
 $t_{30} = t_{60} = t_{85} = 14$ mins

collection of sample products is no longer necessary, the samples are collected in the region where the desired sample is expected to peak. The samples can then be analyzed and those containing lower concentrations of the desired component are pooled and concentrated. This staged sequence cyclic process can be used to concentrate and/or purify desired solutes, even if the solutes exist in trace or high concentration levels.

Figures 8.35 and 8.36 illustrate experimental and theoretical verification of a staged sequence cyclic process. Products high in concentrations of O-Xylene and Anisole are obtained when the one column process was operated with thermal switching periods for all temperatures equal to 10 mins. Figure 8.35 shows a case when there is no reflux. For there to be no reflux, all exiting fluid from the column not taken as product are completely discarded while fresh feed is fed continuously into the column. Since the cycling zone experiments have helped to establish the times at which O-Xylene and Anisole peaked at T_2 and T_3 , for a given thermal switching period, a manual or automatic sampling system provides the means by which sample products are withdrawn. At 60°C , the steady state concentration of O-Xylene and Anisole are 1.22 and 0.76 respectively and that of Anisole and O-Xylene at 85°C are respectively 1.32 and 0.99. At 85°C , one can see that the concentration of O-Xylene is about the feed concentration. This is the result of the O-Xylene peaking with Anisole peak (See Figure 8.30) when Anisole is withdrawn. This phenomena (concentration of O-Xylene close to feed concentration) can also be seen from Figure 8.36. Figure

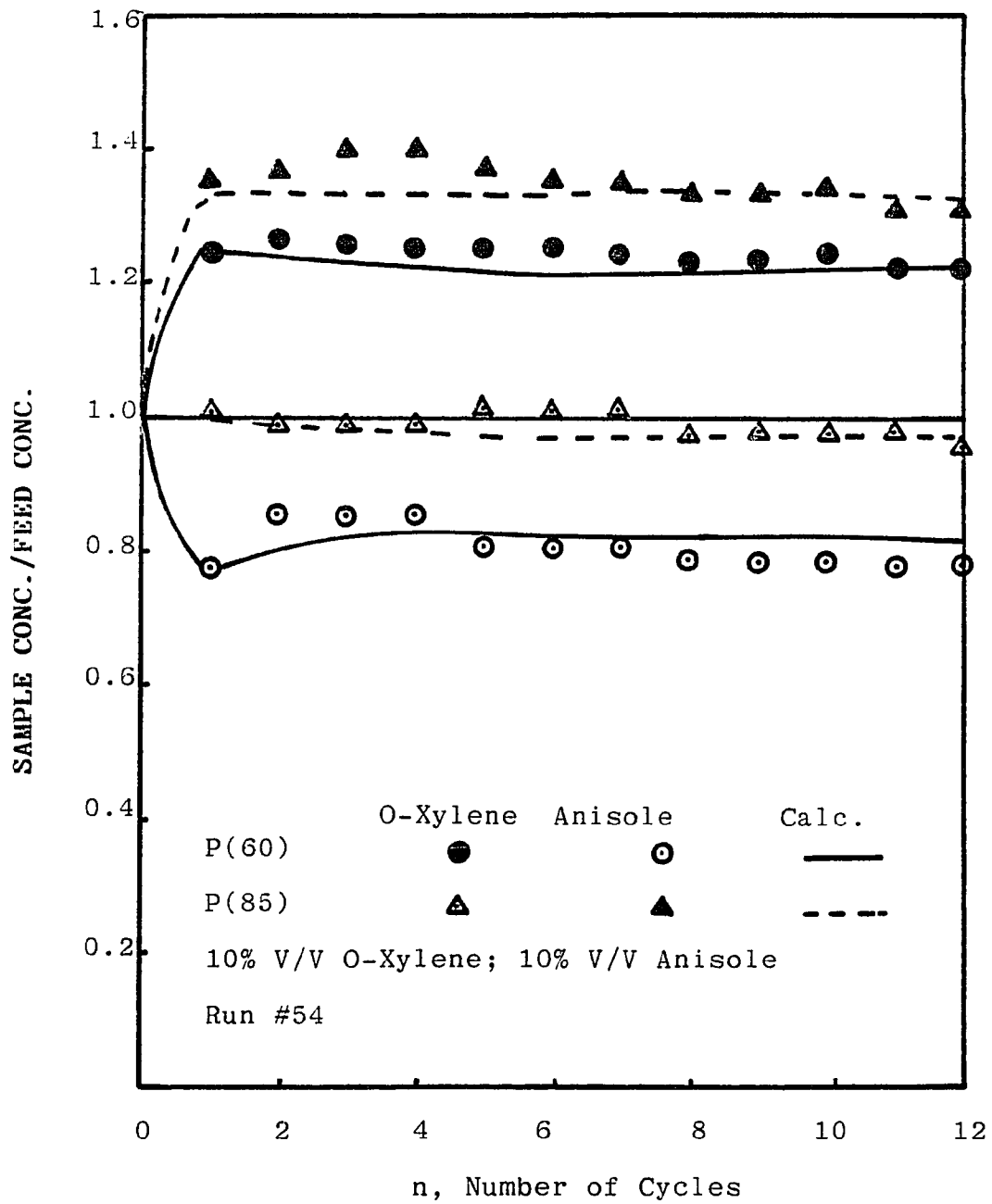


FIGURE 8-35 ONE COLUMN STAGED SEQUENCE - RECYCLE RATIO = 0.0

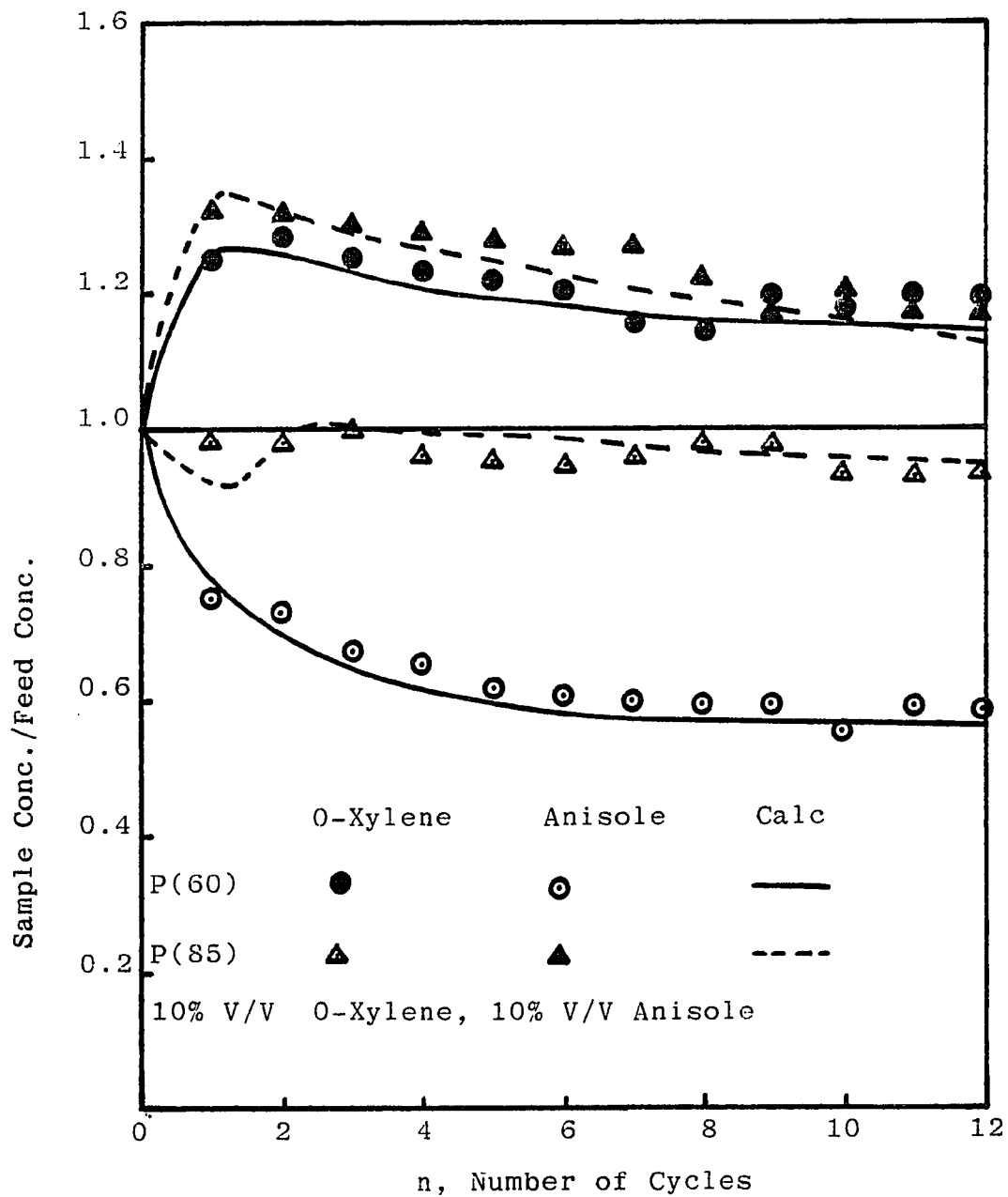


FIG. 8-36 ONE COLUMN STAGED SEQUENCE -- RECYCLE RATIO = 1

8.36 shows the effect of complete recycle (or reflux) on separation. The fresh feed is mixed with the portion of the effluent not withdrawn as product and fed to the column. The fresh feed is now used as a make-up fluid to compensate for the product withdrawn. The product concentrations from these experiments are qualitatively and quantitatively in agreement. In view of the fact that these concentrations represent average values over a given period of time, the separation is comparatively good relative to separations normally obtained with conventional parametric pumping. Large separations could be obtained if the concentration bands in very concentrated regions for O-Xylene and Anisole at 60°C and 85°C are taken as products.

MULTICOLUMN STAGED SEQUENCE CYCLIC PROCESS

Figures 8.37 through 8.54 show the theoretical results of the multicolumn staged sequence cyclic process. It is necessary to present a large number of figures so as to be able to see the effect of all the variables. All of the theoretical results were obtained via the numerical solution of the transport equations with finite mass transfer and non linear equilibria.

Figures 8.37 and 8.38 show the transient product concentrations taken at T_2 and T_3 respectively for a system with $\alpha = 1.0$ and $P_T = P_B = 0.20$. By nature of the column arrangements, non-symmetrical flow rates results in the three columns per stage. The column at T_3 always has less material in it per a given stage. Figure 8.37 show a modest separation when the columns are

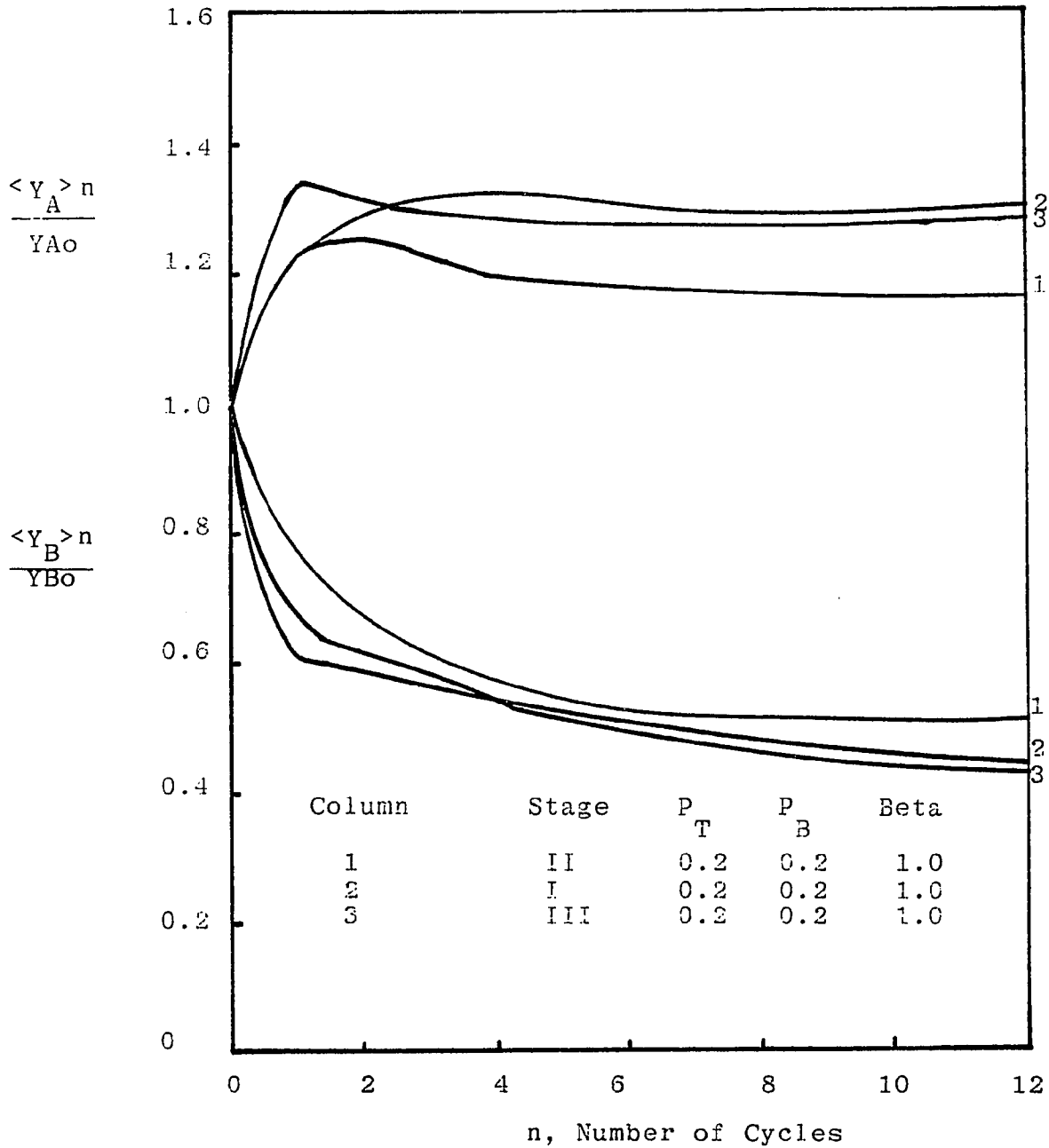


FIGURE 8.37 PRODUCT CONCENTRATION AT T_2 ($T_1 < T_2 < T_3$)
 $Q = 25$, TIME = 15, NNZ = 29, H = 90
 $Y_{Ao} = 0.00095$ gmole/cc, $Y_{Bo} = 0.00086$ gmole/cc

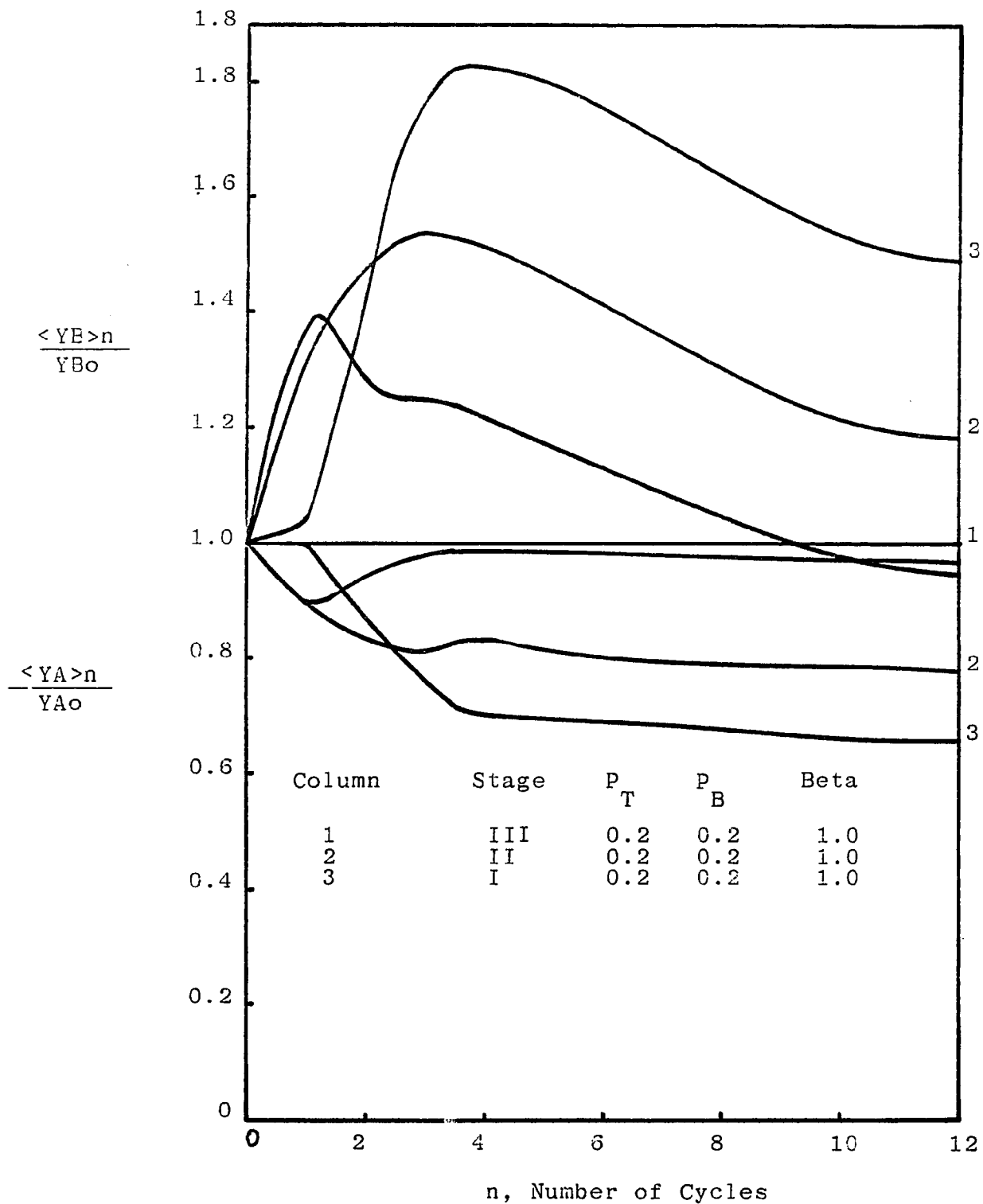


FIGURE 8.38 PRODUCT CONCENTRATION AT $T_3 (T_1 < T_2 < T_3)$, $YBo = 0.00095$ gmole/cc
 $YBo = 0.00086$ gmole/cc $Q = 25$, TIME = 15, NNZ = 29, H = 90

operated for 15 mins per stage, while in Figure 8.38, the phenomena of component A (which in this case will be O-Xylene) with product concentrations close to the feed concentration is again observed. The concentrations of component B (Figure 8.38) show arbitrarily high concentration around the third cycle and dropping off sharply in all the three stages. Since component B is the slower moving component, it tends to concentrate into bands while moving slowly down the column. The sharp concentration rise observed in the first or second cycle is a result of the accumulation of sharp concentration waves moving closely together down the column. As soon as the concentrated solution rich in component B exits the column at T_3 on the third cycle, the concentration on subsequent cycles successively falls till steady state concentration is reached on the twelfth cycle. It can also be seen that the steady state concentrations of components A and B become increasingly reduced with increase in stage, and are almost identical, falling slightly below the feed concentration in Stage III. An obvious reason for this is that at the start of the run, there is tremendous amount of axial dispersion in the T_3 column where product rich in component B is withdrawn due to a decrease in flow rate and thus column displacement.

Figure 8.39 shows the concentration transients for the enrichment components A and B for $P_T=0.200$ and 0.365 (where $P_T+P_B = 0.400$). Component B still exhibited the phenomena of sharp increase and an abrupt decrease in concentration and in some cases the steady state concentration is well below the feed

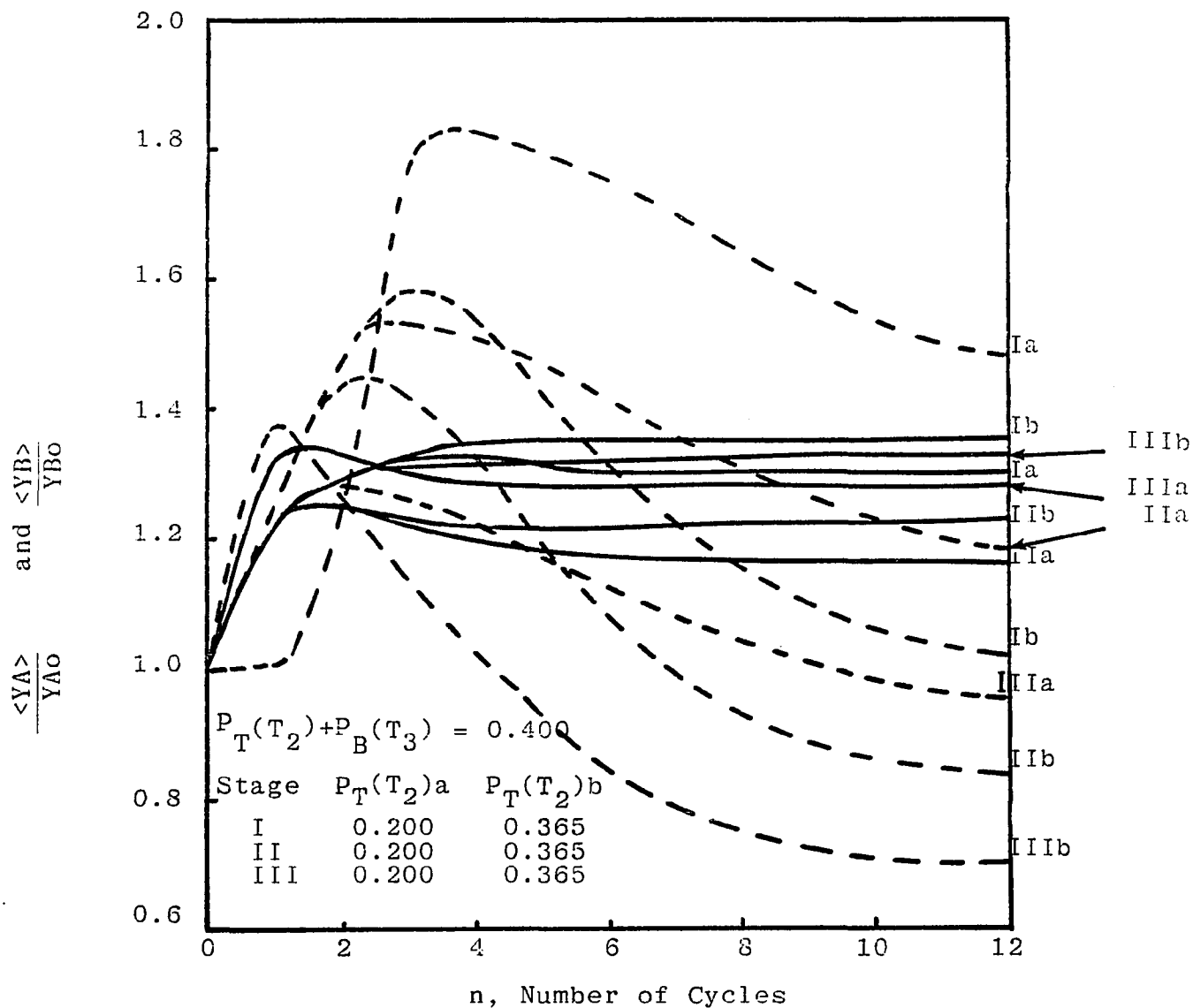


FIGURE 8-39 EFFECT OF PRODUCT WITHDRAWAL RATE ON CONCENTRATION TRANSIENTS FOR BETA = 1.0, Q = 25
 TIME = 15, NNZ = 29, H = 90, YAO=0.00095,
 (——), COMPONENT A, (----) COMPONENT B

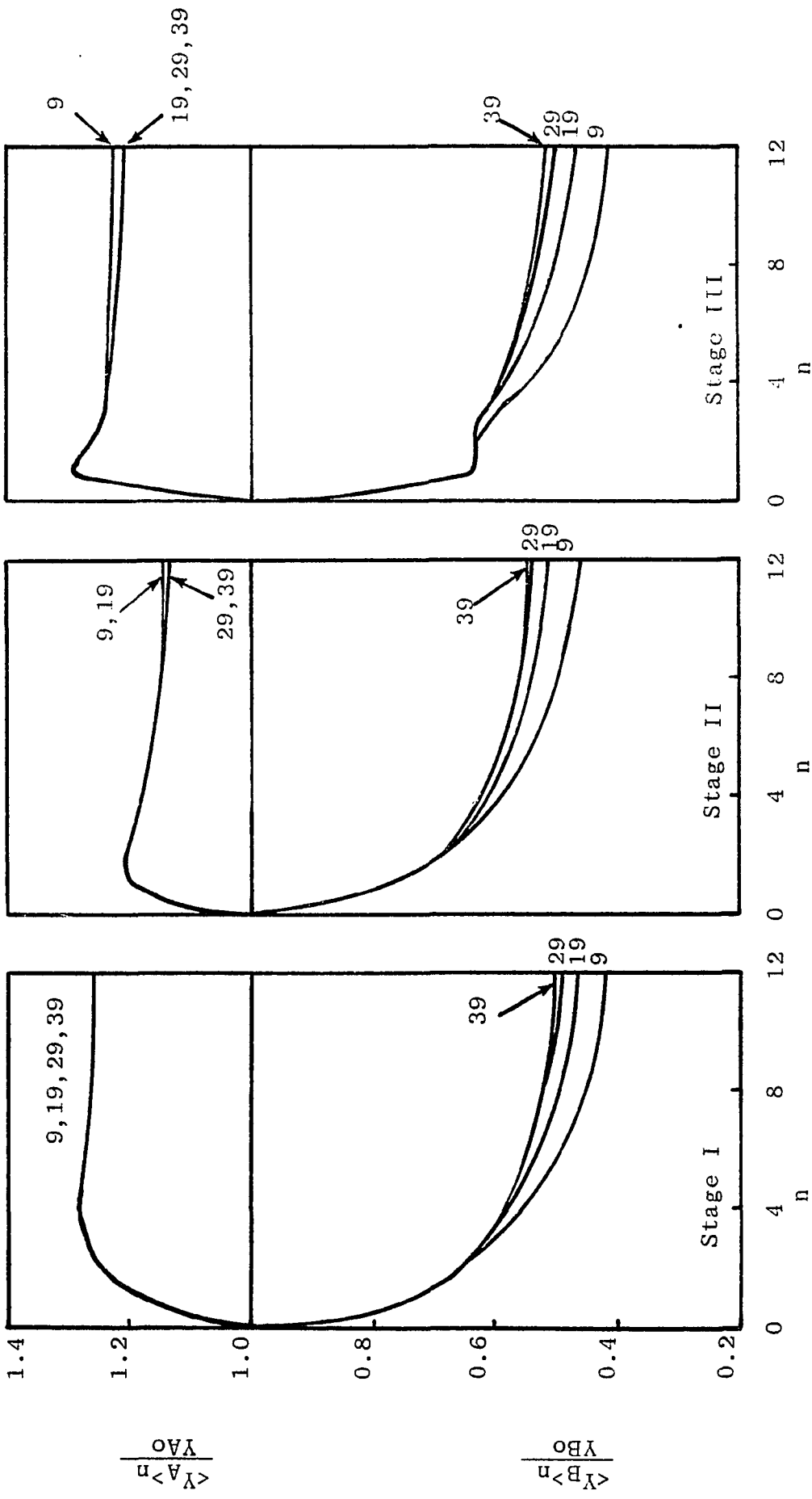


FIGURE 8-40 EFFECT OF NUMBER OF CELLS ON CONCENTRATION TRANSIENTS FOR COMPONENTS A & B
 AT T_2 , $H=90\text{cm}$, $\text{TIME}=10.0$ mins, $P=0.20$, $P_\eta=0.20$, $Q=25$ Beta=1.00, $Y_{A0}=0.00095$
 gmoles/cc and $Y_{B0}=0.00086$ gmoles/cc

concentration (about 0.75) especially in Stage III with $P_B=0.035$. The reason for this extremely low value is that the quantity withdrawn per stage is so small that the bulk of component B remains virtually in the column since component B is more strongly adsorbed and therefore with slower relative velocity (not always the case). The concentrations of component A show no unusual behavior. Figure 8.40 shows the effect of the number of cells on the transient concentration. In this figure, only the products withdrawn at T_2 (i.e. high concentration of component A and low concentration of component B). It can be seen that the number of cells has relatively no effect on the enrichment of component A, but a significant effect on the depletion of component B. In all the three stages, arbitrarily low concentration of component B is produced with a decrease in the number of cells. When the columns are divided into fewer number of cells, dispersion and axial mixing is introduced and the dilute materials are more affected since they are more sensitive to dispersive and various phenomenological forces occurring in the columns. The effect is more pronounced as dilute material is being produced as the number of cycle is increased. However, increasing the number of cells decreases the sensitivity, such that for $NNZ=29$ and 39 , the concentration of component B is virtually the same. The mathematical method of determining the number of cells necessary for stability in numerical computation was not used since it is just as easy to determine it by trial and error. Above and below the optimum number of cells, the computation time could be enormous. Above

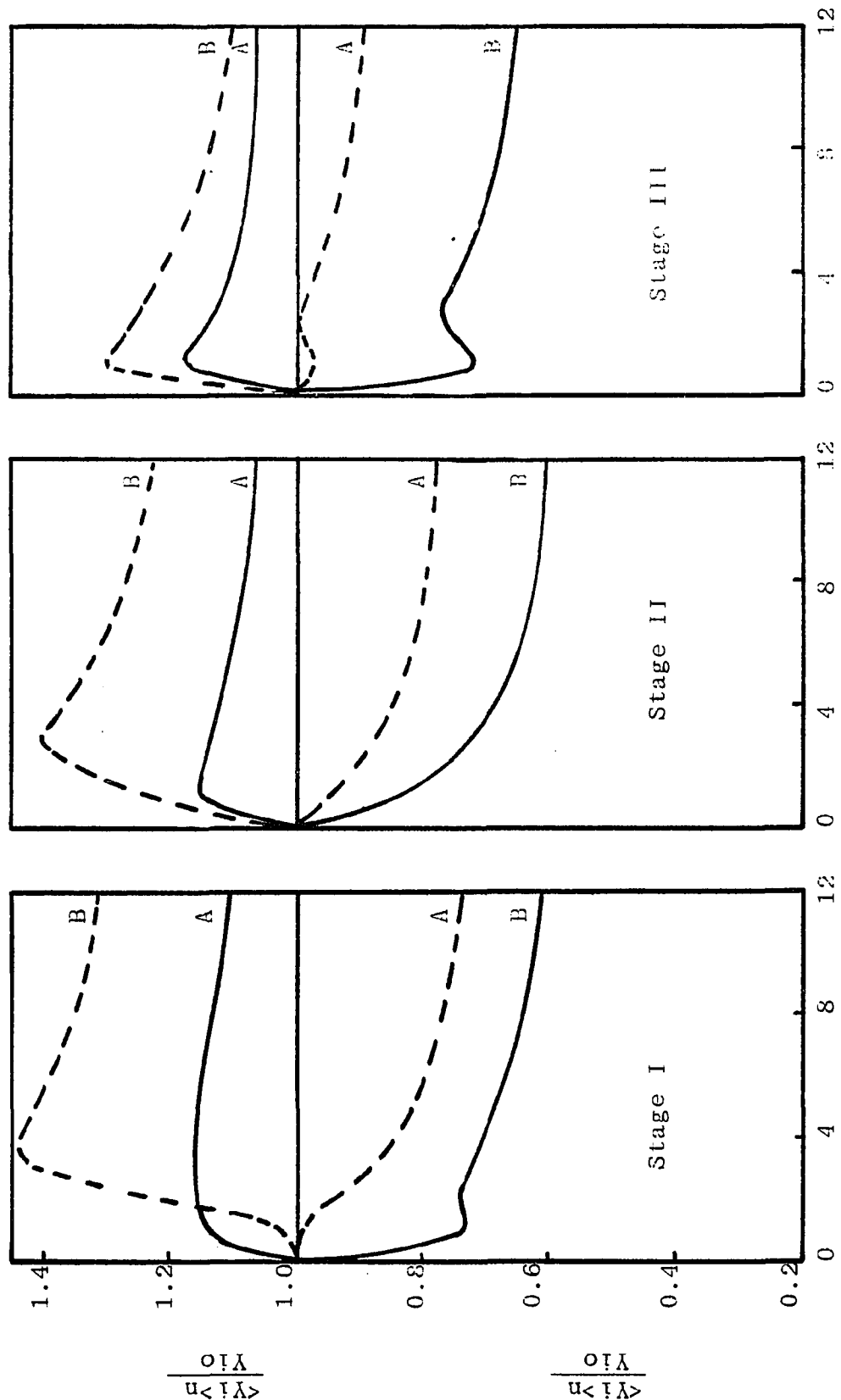


FIGURE 8-41 CONCENTRATION TRANSIENTS FOR COMPONENTS A & B FOR $H = 75$ cm
 TIME = 5.00 mins, $P_T = 0.20$; $P_B = 0.20$, BETA = 1.00, $Y_{A0} = 0.00095$ gmole/cc
 $Q = 25$ and $Y_{B0} = 0.00086$ gmole/cc (-----) at T₂, (----) at T₃

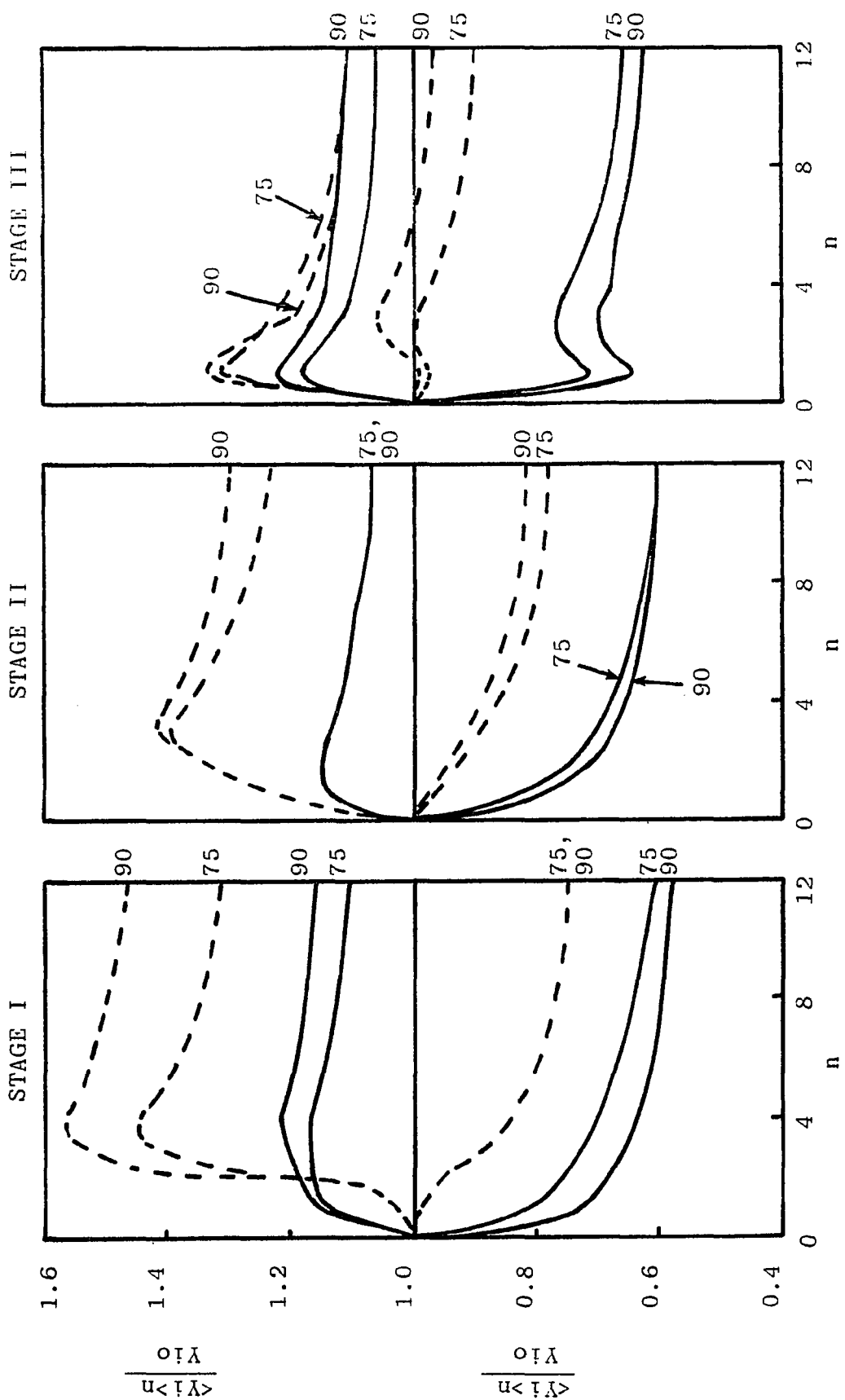


FIGURE 8-42 EFFECT OF COLUMN HEIGHT ON CONCENTRATION TRANSIENTS FOR COMPONENTS A & B
 TIME = 5.00 mins, $P_T = 0.20$, $P_B = 0.20$, Beta = 1.00, $Y_{A0} = 0.00095$ gmole/cc
 $Q = 25.0$ cc and $Y_{B0} = 0.00086$ gmole/cc (—) at T_2 , (-----) at T_3

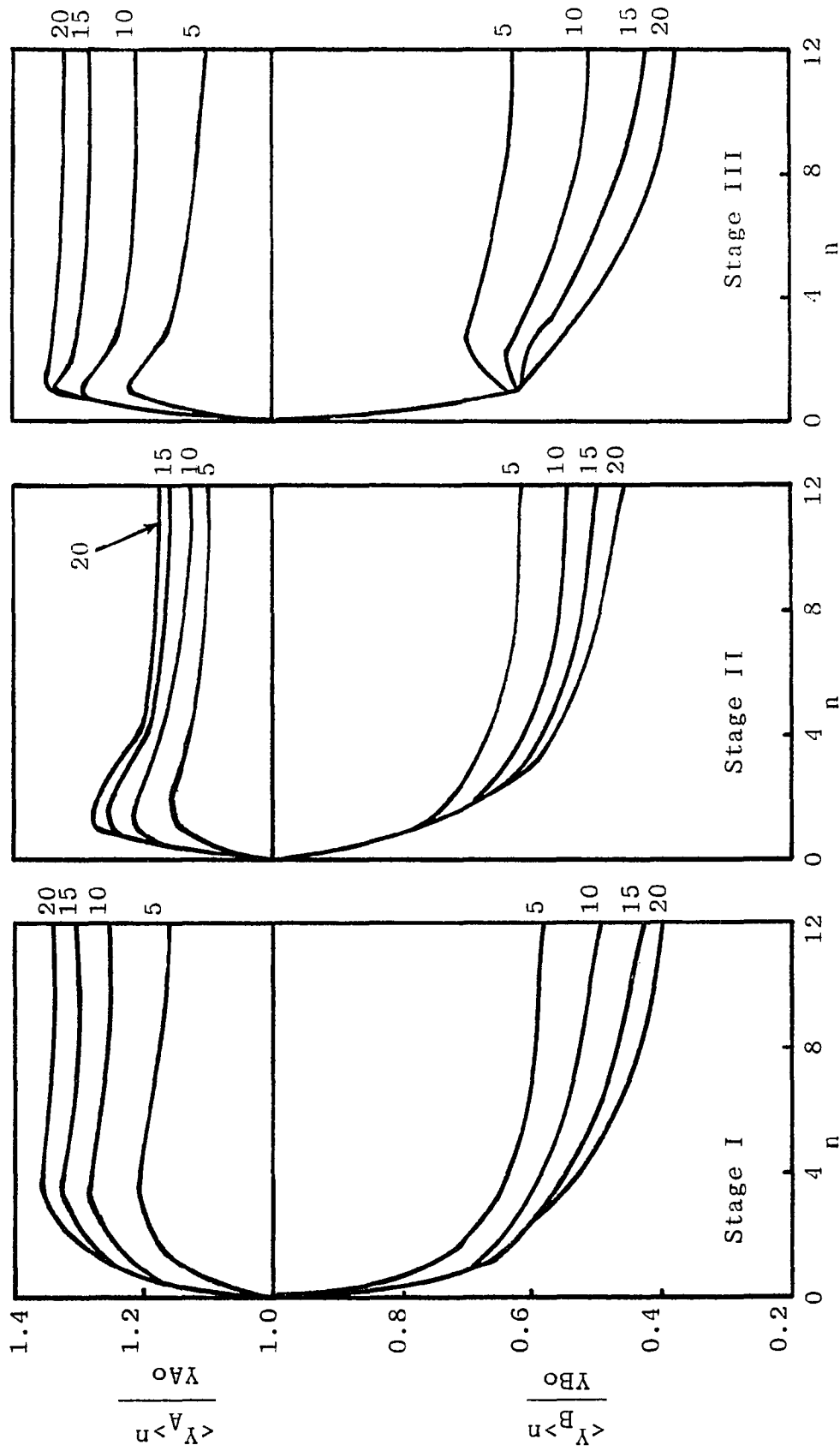


FIGURE 8.43 EFFECT OF STAGE TIMES ON CONCENTRATION TRANSIENTS FOR COMPONENT A & B AT T_2 , $NNZ = 29$, $H = 90.0$, $P_T = 0.20$,

$P_B = 0.20$, $BETA = 1.00$, $Y_{Bo} = 0.00095$, $Q = 25 Y_{Co} = 0.00086$

the optimum, the column concentrations are unnecessarily computed for more cells than required while below the optimum, the convergence is slow.

Figure 8.41 and 8.42 show the effect of column height on concentration transients for both components A and B. Figure 8.41 shows concentration profiles for components A and B for $H = 75.00$ cm, while Figure 8.42 shows the relative comparison of the concentration profiles for both components for process operated with $H = 75.00$ cm and 90.00 cm. All the rest of the simulation was done with $H = 90.00$ cm since the column height used for the experimental part is 90 cm. Overall, simulation with $H = 90.00$ cm produced better separation. The height of the column only affected the separation in Stage I and little or no effect in Stages II and III. Figures 8.43 and 8.44 illustrate the effect of stage duration time on the production of components A and B. From Figure 8.43, separation in all the three stages increase with increase in stage duration time. This theoretical result agrees well with experimental observation. In the one column cycling zone experiment, it was seen that as the thermal switching period (See Figure 8.30 and 8.31) is increased from 10.0 minutes to 14 minutes, the O-Xylene peak which in this case would be component A separates better from Anisole. At $t_{30}=t_{60}=t_{85}= 10$ mins, (Figure 8.30) the second O-Xylene peak is burried under the Anisole peak, while at $t_{30}=t_{60}=t_{85} = 14$ mins (Figure 8.31), the separability of this second peak was improved. In the case of the simulation, the longer the stage

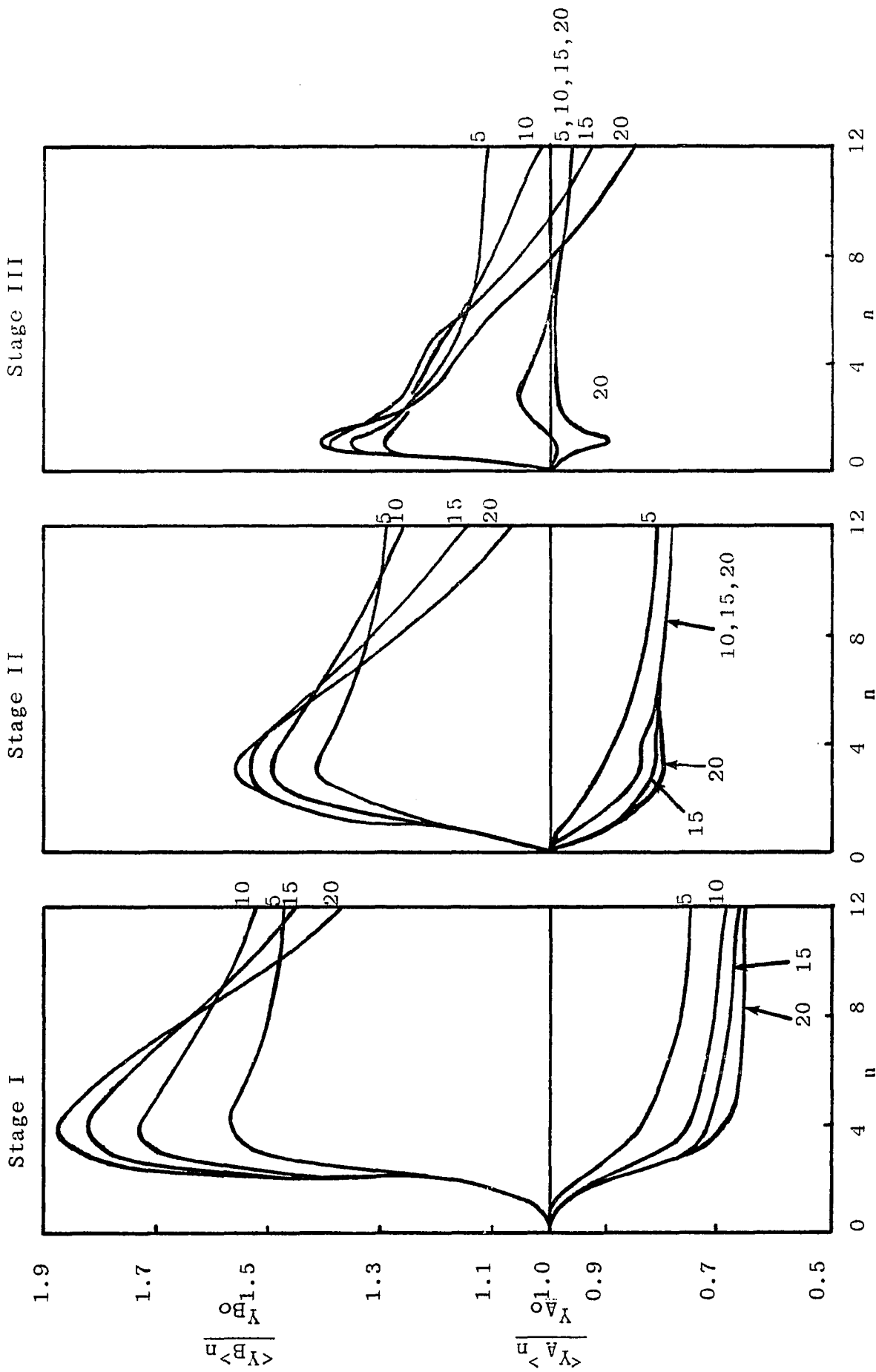


FIGURE 8-44

EFFECT OF STAGE TIMES ON CONCENTRATION TRANSIENTS FOR COMPONENT A & B

AT T_3 . $NNZ=29$, $H=90.0\text{cm}$, $P_T=0.20$, $P_B=0.20$, $P_B=0.20$, $\beta_B=0.00095$ gmole/cc
 $Y_{Co}=0.00086$ gmole/cc and $Q=25$

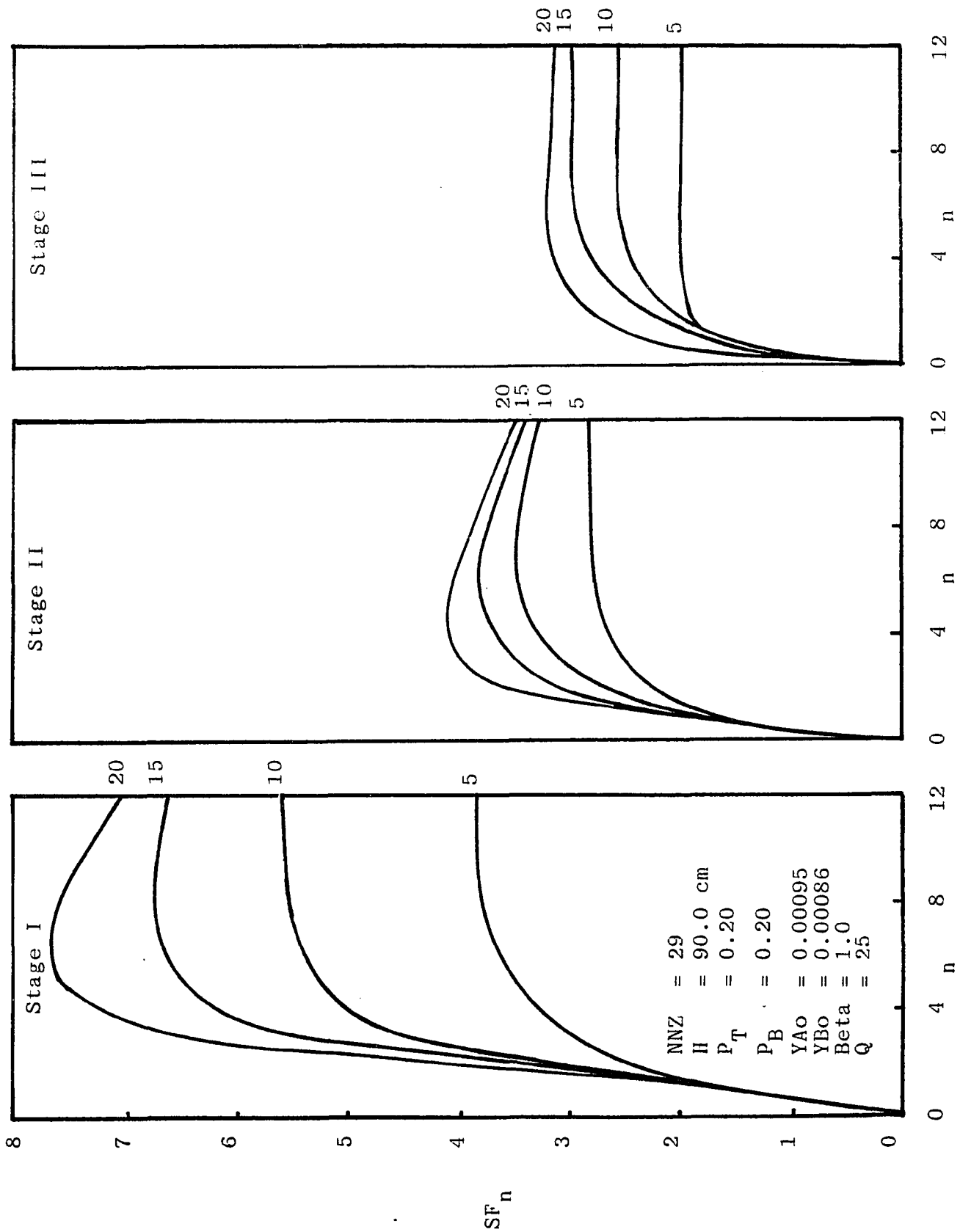


FIGURE 8-45 EFFECT OF STAGE TIME ON SEPARATION FACTOR

duration time, the two peaks observed in the experiment may tend to exit the column as one concentrated peak hence the increase in the concentration of component A (Figure 8.43) with stage duration time. But the enrichment of component B (Figure 8.44) at various stage duration time shows that the steady state concentration is drastically reduced with stage duration above 10 mins. The highly concentrated wave fronts of component B is essentially withdrawn as product at or about the fourth cycle for Stage I, third cycle for Stage II and second cycle for Stage III. After the high concentration bands are withdrawn, subsequent cycles consists of less concentrated withdrawn in component B, especially the stage duration time well above 10 minutes. The separation factors for the various stage duration is shown in Figure 8.45. The separation factor is defined as follows:

$$SF_n = \left[\frac{\langle y_A \rangle_n / y_{Ao}}{\langle y_B \rangle_n / y_{Bo}} \right]_{T_2} \cdot \left[\frac{\langle y_B \rangle_n / y_{Bo}}{\langle y_A \rangle_n / y_{Ao}} \right]_{T_3} \quad (8.1)$$

or at steady state,

$$SF_{ss} = \left[\frac{\langle y_A \rangle_{\infty} / y_{Ao}}{\langle y_B \rangle_{\infty} / y_{Bo}} \right]_{T_2} \cdot \left[\frac{\langle y_B \rangle_{\infty} / y_{Bo}}{\langle y_A \rangle_{\infty} / y_{Ao}} \right]_{T_3} \quad (8.2)$$

The separation factor obtained from Stages II and III are almost equal and much less than the separation factor obtained from Stage I. If the separability is determined from the separation factor, one would at first glance consider stage duration time of 20 minutes as the most desirable. The separation factor

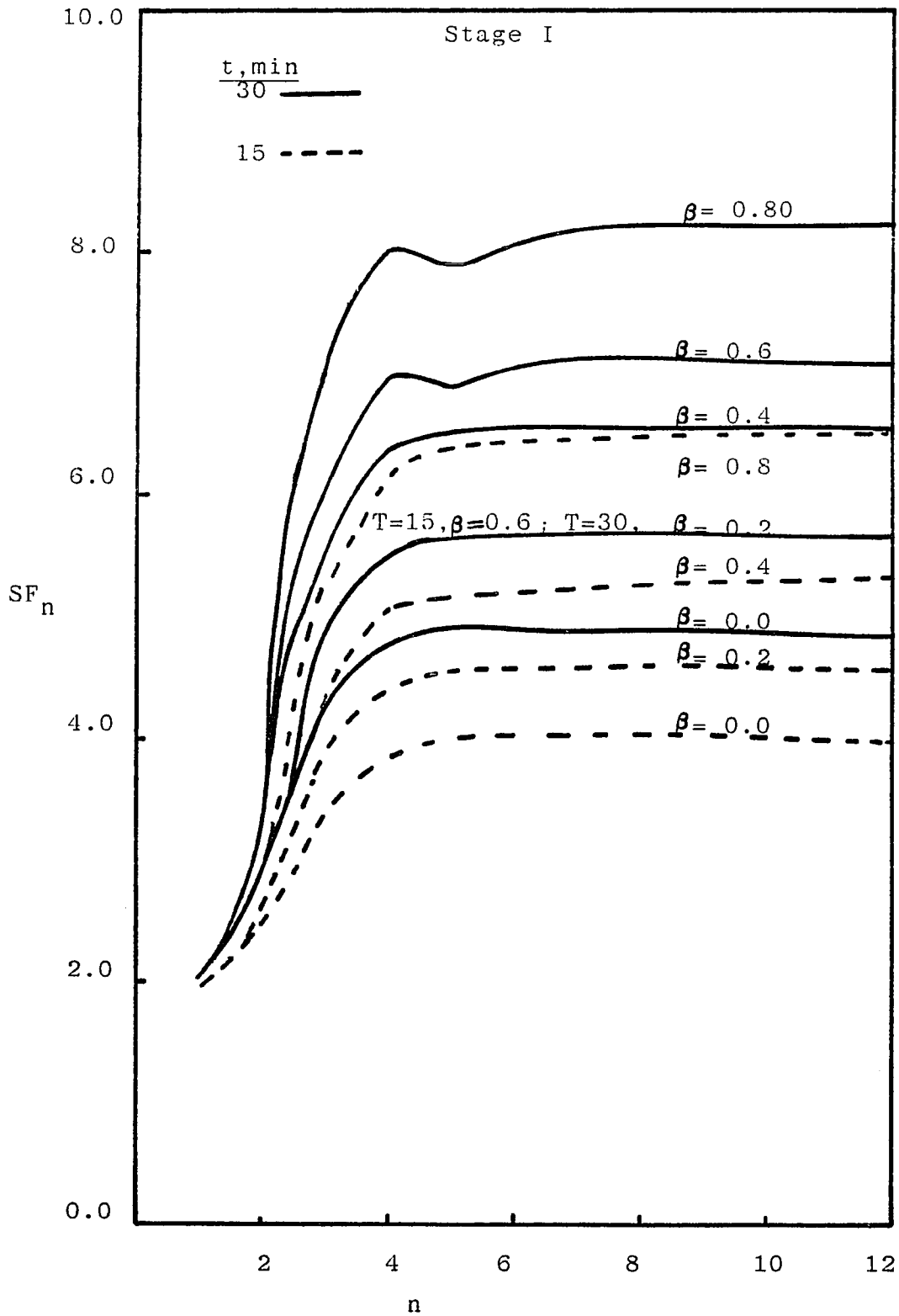


FIGURE 8-46 EFFECT OF RECYCLE RATIO ON SEPARATION FACTOR

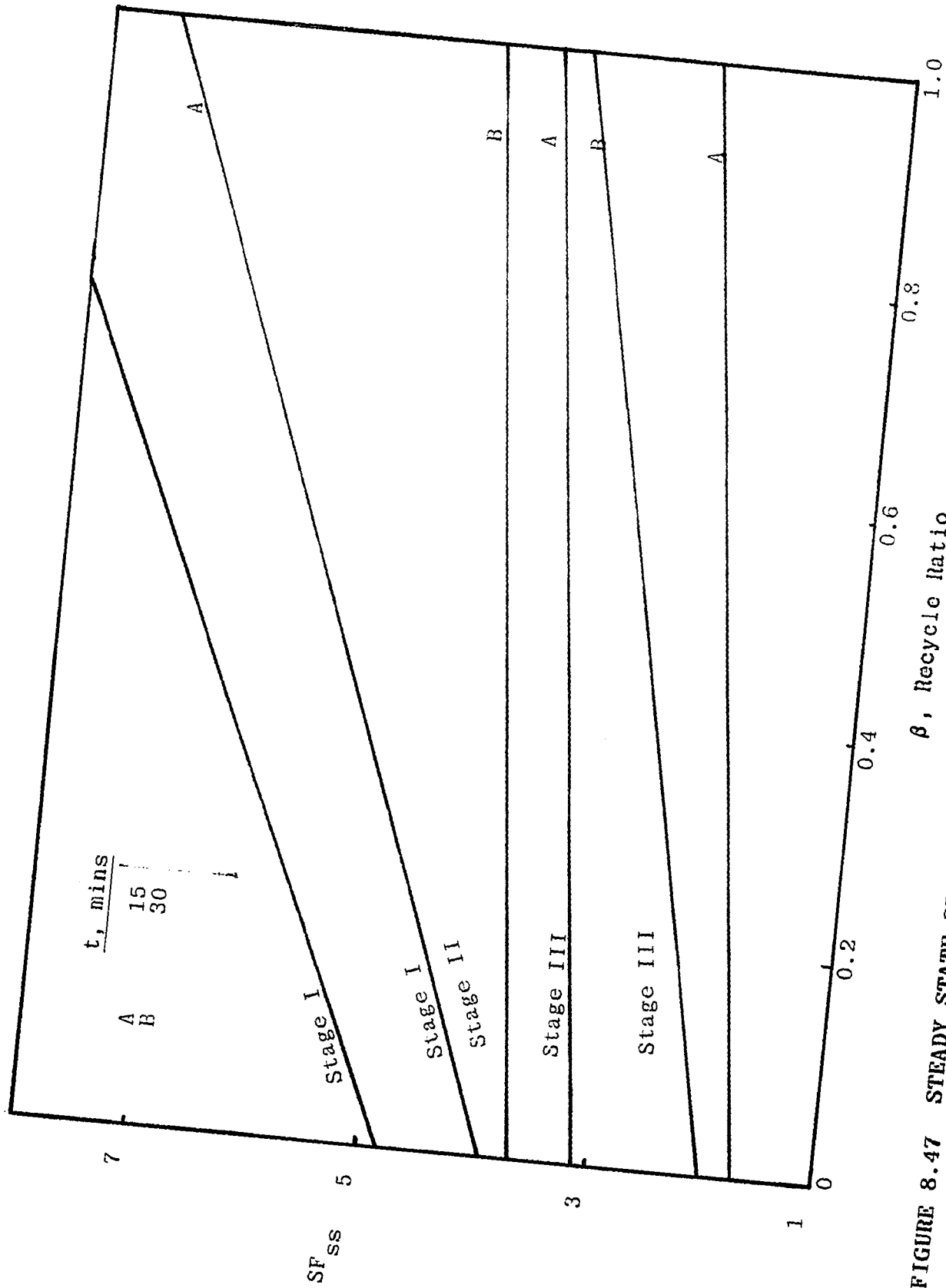


FIGURE 8.47 STEADY STATE SEPARATION FACTOR VERSUS RECYCLE RATIO

especially of a two component system determines how well separated one component is compared to another, but not on the enrichment of the two components. If a stage duration time of 20 minutes is chosen, at steady state, highly concentrated A will be produced and not so concentrated B will be produced, but if 10 or 15 minutes is used as the stage duration time, a modest enrichment of both components A and B will be produced.

Figures 8.46 and 8.47 show the effect of recycle on separation factors for $t = 15$ and 30 minutes. Again the simulation for $t = 30$ mins. produces higher separation factors, not because longer stage duration time results in higher recoveries of both components A and B but because separation factor is in effect a measure of separability. In this case, high recovery of component A is achieved at the expense of component B. Figure 8.46 shows only the separation factor obtained in Stage I, but the profiles of the separation factors from Stages II and III are similar but slightly lower. This fact can be seen clearly from Figure 8.47. The steady state separation factors as found in all of the three stages for $t = 15$ and 30 minutes show that separation increase with increase in recycle ratio. In some cases, such as in Stages I and II, the steady state separation for $t = 15$ and 30 mins are parallel. Figures 4.48 and 4.49 illustrate the effect of product withdrawal rate on separation. Equal product withdrawal rates are used since we already saw the effect of unequal product withdrawal rate from Figure 8.39. It should be remembered that the size of products withdrawn determines the movement of concentration waves (penetration distances of both

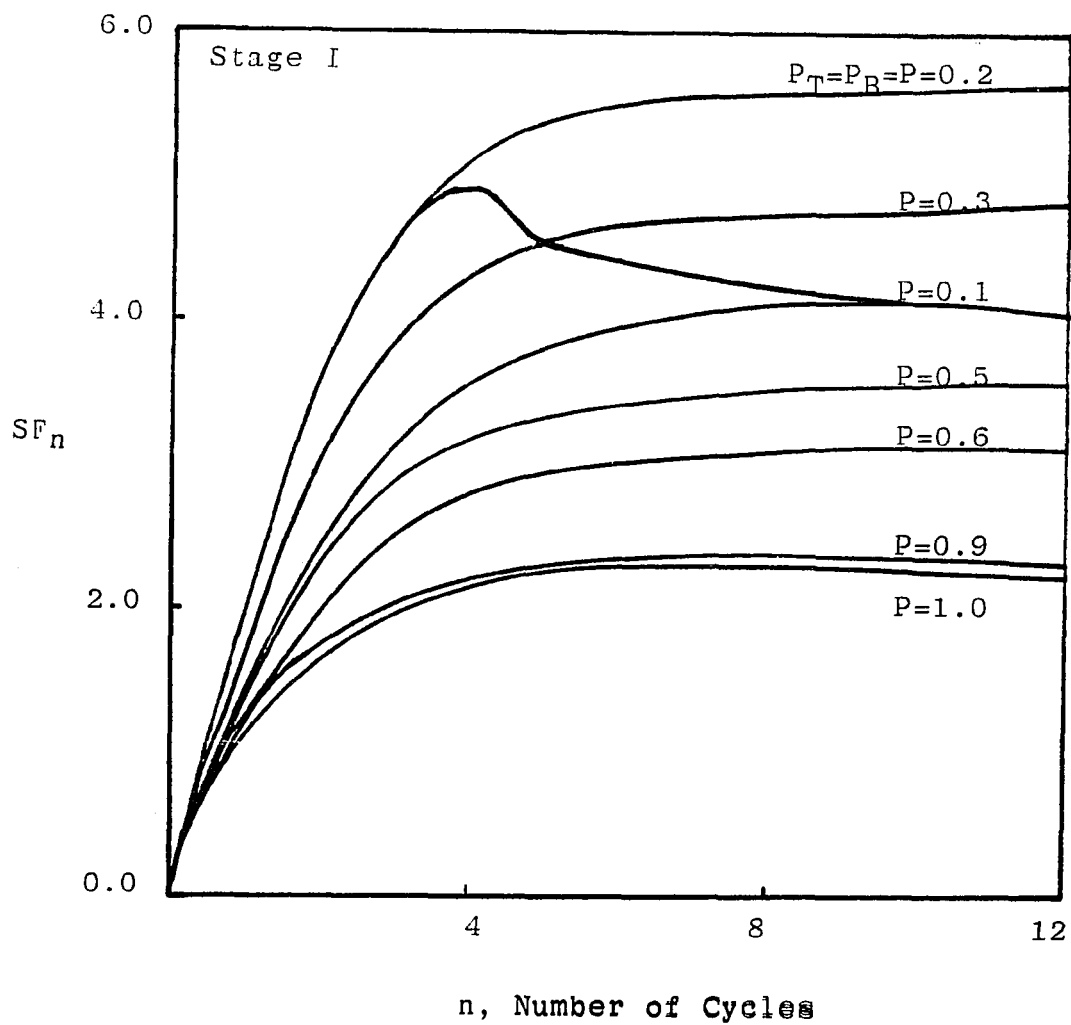


FIGURE 8-48 EFFECT OF PRODUCT WITHDRAWAL RATE ON SEPARATION

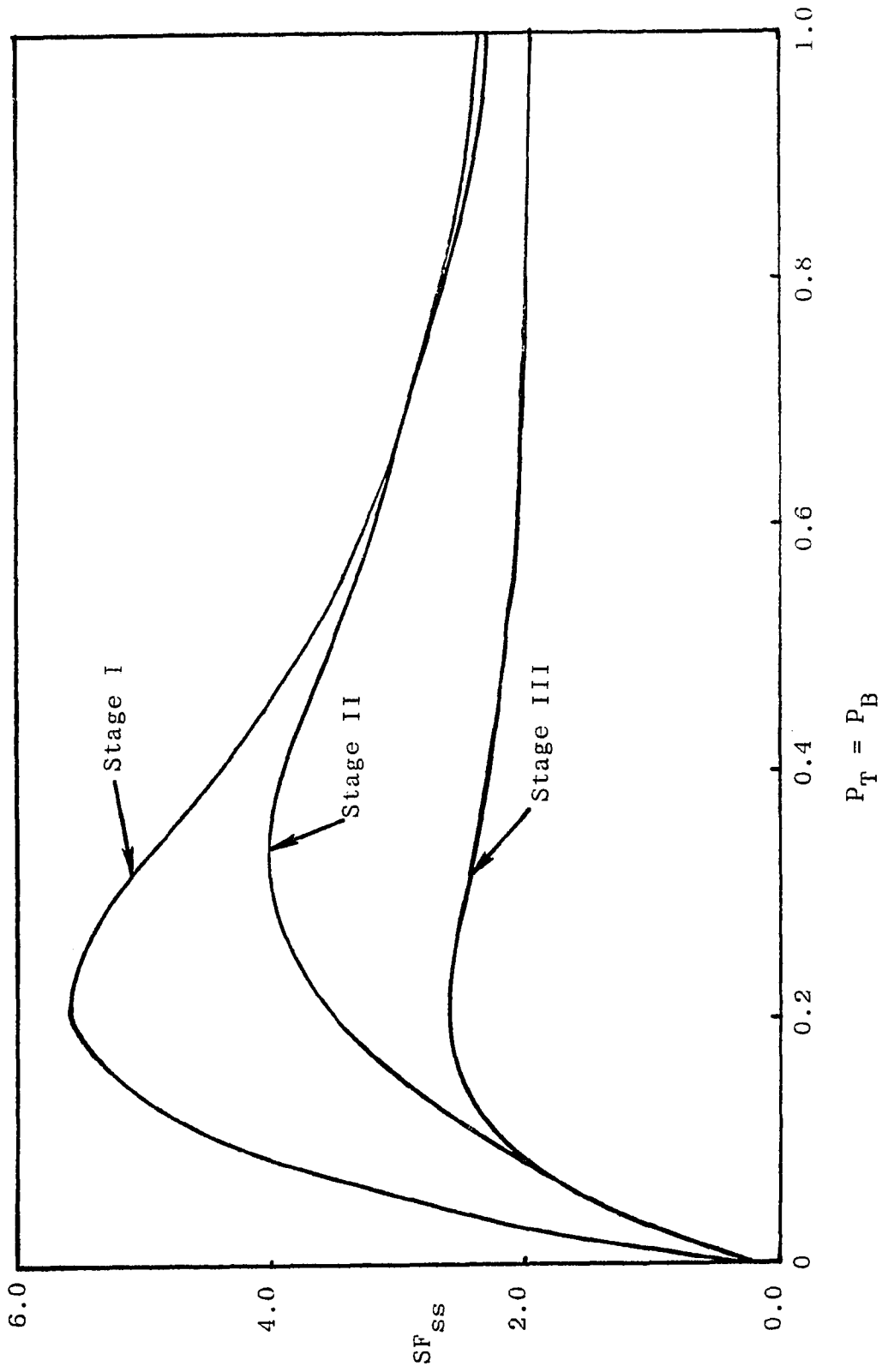


FIGURE 8-49 EFFECT OF PRODUCT WITHDRAWAL RATE ON STEADY STATE SEPARATION FACTOR

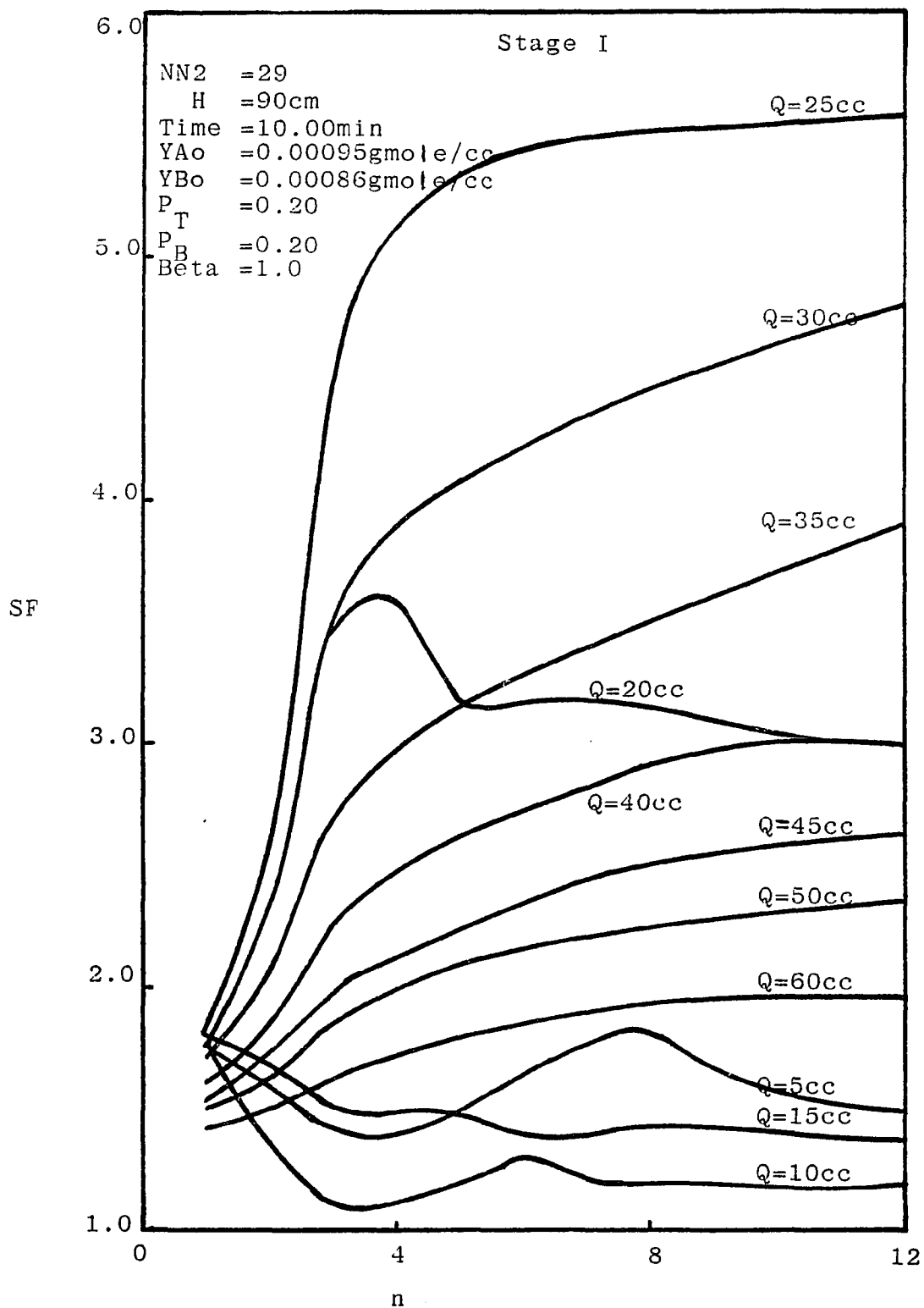


FIGURE 8-50 EFFECT OF COLUMN DISPLACEMENT ON SEPARATION FACTOR

components) that move through the column. Lets consider an extreme case where $P_T=P_B=P=1.0$, that means that the feed introduced into the column and therefore the products withdrawn is the same, size as the amount of displaceable volume in the column, meaning that the sample withdrawn goes through only one series of temperature step inputs. An optimum product withdrawal rate exist for which the best separation can be obtained. This is clearly illustrated in Figure 8.49 that maximum separation can be obtained in Stages I and III when $P_T=P_B=P=0.2$ while the same is true for Stage II when $P_T=P_B=P=0.3$. The optimum value of $P_T=P_B=0.2$ was used in most of the theoretical simulation. The existence of this optimum value of $P_T=P_B$ means that the fluid mixture has undergone optimum series of temperature inputs to yield optimum separation.

Figures 8.50 and 8.51 show the effect of column displacement on separation factors. At extremely low values of Q , the separation factor and thus the solute concentrations are irregular and oscillatory. At very high values of Q , the separation is low. An optimum value of Q is observed. This optimum value is $Q=25\text{cc}$ and with this value, a maximum separation can be obtained. The column void volume is between 25 cc to 29cc depending on the accuracy to which to column is packed. This optimum value of Q can be clearly seen from Figure 8.51. At extremely low values of Q , the fluid and therefore the concentration waves spend longer time in the column and they undergo various temperature changes. In the process of this repeated

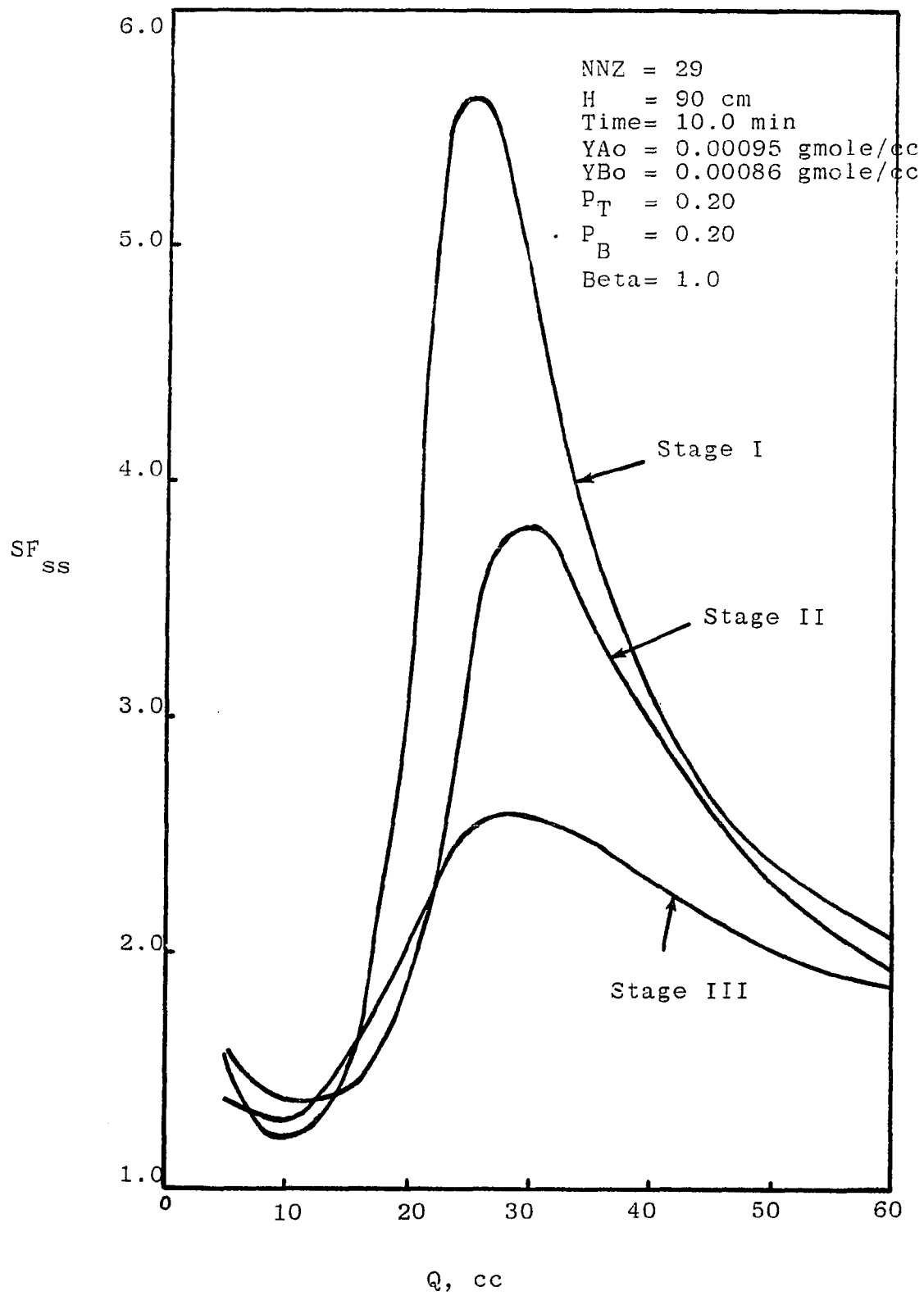


FIGURE 8.51 STEADY STATE SEPARATION FACTOR VERSUS COLUMN DISPLACEMENT

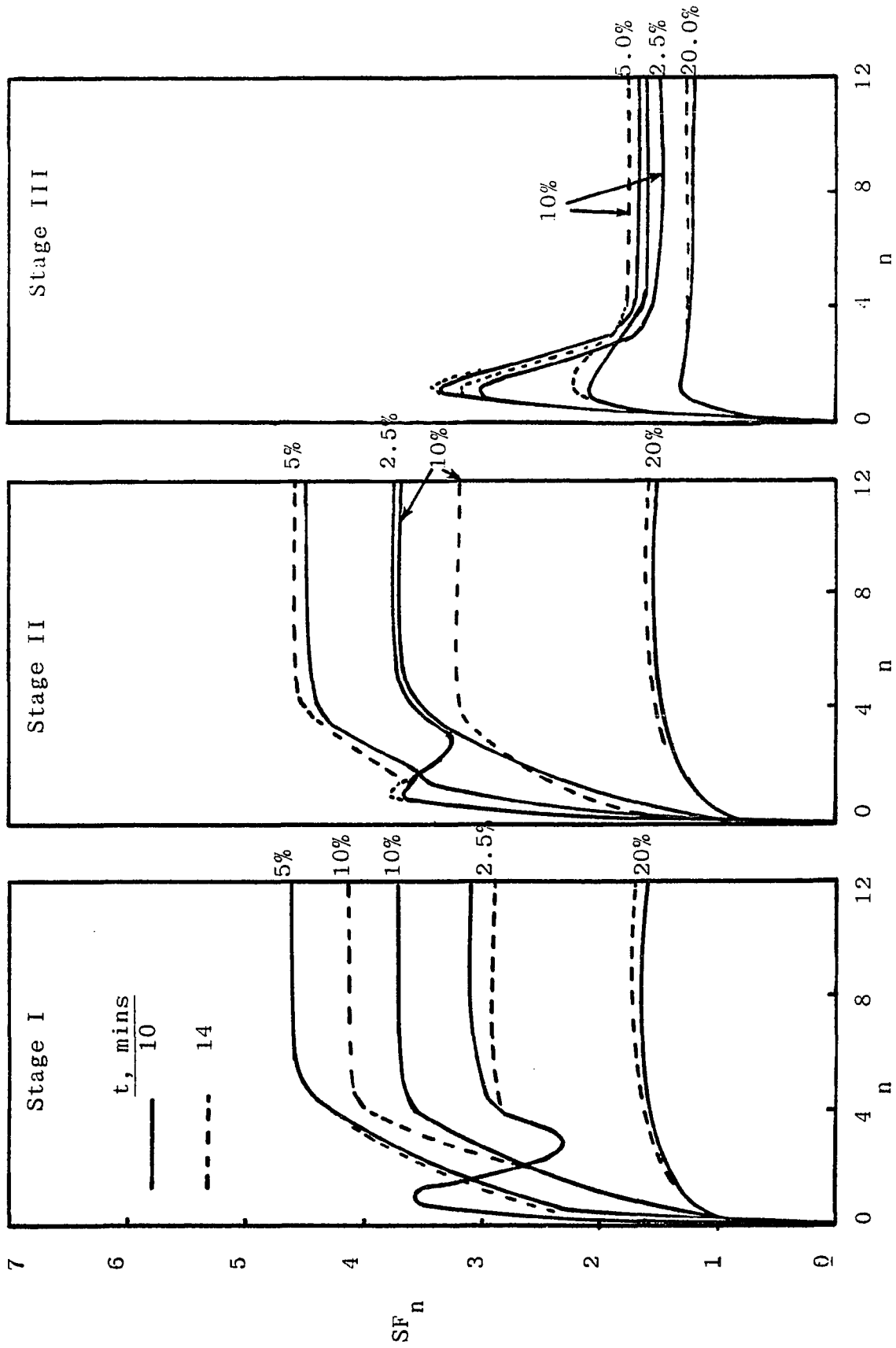


FIGURE 8.52 EFFECT OF CONCENTRATION ON SEPARATION FACTOR, RECYCLE RATIO = 0.0

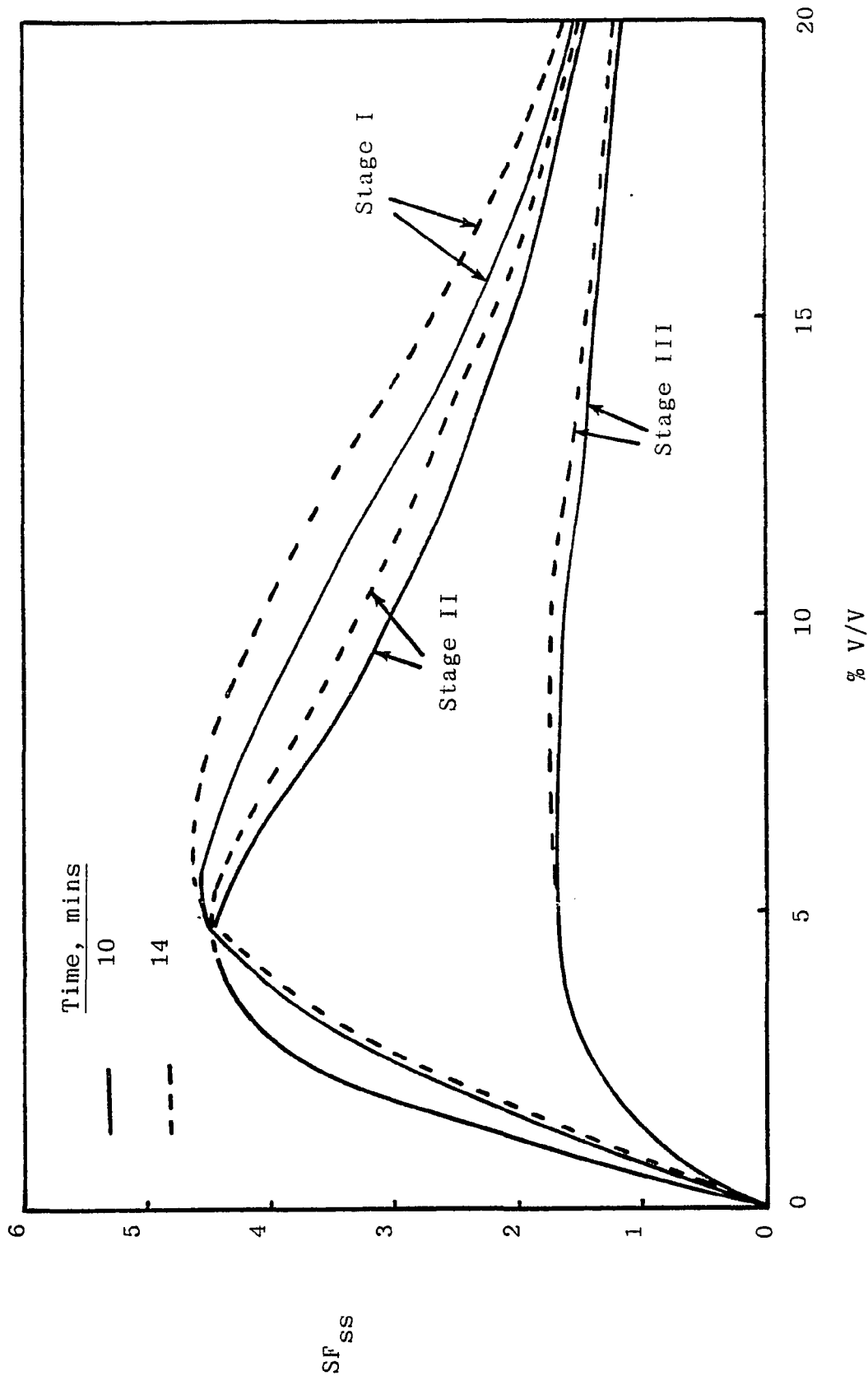


FIGURE 8.53 EFFECT OF CONCENTRATION ON STEADY STATE SEPARATION FACTOR

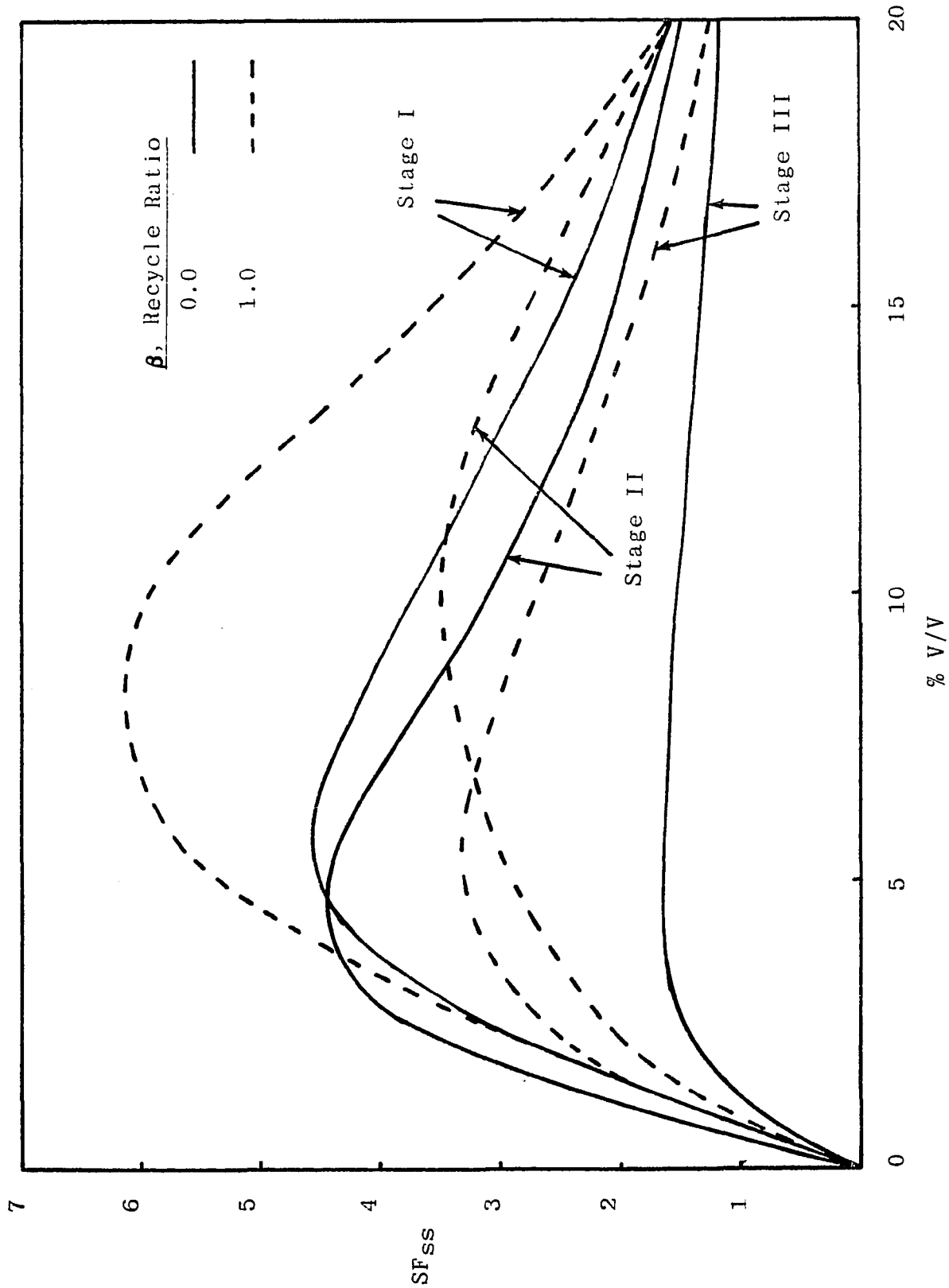


FIGURE 8.54 EFFECT OF CONCENTRATION ON STEADY STATE SEPARATION FACTOR FOR RECYCLE RATIO = 0.0 AND 1.0

temperature change the majority of the concentration waves cancel each other out with only a few exceptions. At very large values of Q , more fluid mixtures (much more than the void volume of the column) are passed through the column and that again reduces the concentration. Figures 8.52 to 8.54 illustrate the effect of feed concentration on separation for $t = 10$ and 14 mins and recycle ratios of 0.0 and 1.0 . It can be seen that 5% V/V of feed for both components gives better separation. At extremely high feed concentration such as 20% V/V, the separation is drastically reduced since the condition of extreme non-ideality and non-equilibrium conditions is approached. At low feed concentrations such as 2.5% V/V, most of the material are adsorbed in the column since the active sites in the solid phase are relatively unoccupied. It can also be seen from Figure 8.54 that a recycle ratio of 1.0 would give better separation in Stage I in comparison with recycle ratio of 0.0 for the same reasons given earlier during the discussion of recycle ratio on separation.

CHAPTER 9

CONCLUSIONS AND RECOMMENDATIONS

In this dissertation the emphasis has been on the design of a fixed bed adsorption column, development of a parametric pumping process for the purification of multicomponent mixtures in dilute solutions, and on the design of a cyclic process (an alternative to parametric pumping, cycling zone adsorption, or simulated moving bed) suitable for the continuous fractionation of hydrocarbon mixtures for operation in the direct thermal mode.

Various analytical solutions of a fixed-bed sorption column for the prediction of effluent concentrations of each species in both the solid and liquid phases as a function of column position and time space were derived. These analytical solutions were based on the mathematical description of the complete and simplified models. The solution of the complete model was based on various interfacial phenomena subject to pertinent initial and boundary conditions and linear equilibrium distribution, while the simplified model was based on the premise that, in the rate expression, transport resistances in the fluid phase around the particle dominate.

Effluent concentrations as a function of column position and time were obtained via the simplified model. The theoretical calculations showed that, at slow mass exchange, the concentration peaks are sharp and tall, and as mass exchange is increased, the peak shape became broader with decreasing height.

Sharper peaks were also observed with an increase in equilibrium constants.

A multicolumn staged sequence cyclic process for the continuous fractionation of multicomponent fluid mixtures has also been modeled. Experimental data retrieved from a single column staged sequence cyclic process (employing o-xylene-anisole-n-heptane on silica gel) were used for the simulation of the multicolumn cyclic process. The separation of solutes from dilute and concentrated multicomponent solutions were predicted by computer calculations and numerical solutions of the equations of continuity. This mathematical model assumed a finite rate of mass transfer and nonlinear equilibria of individual solutes. The computed concentration profiles agreed with the experimental results. The following parameters affecting the separations were theoretically optimized: number of cells (plates), height of the columns, stage duration time, product withdrawal rates, recycle ratio (reflux ratio), the solute concentrations in the feed, and column displacement volume. The separability of solutes depends functionally on all of the variables. The optimum values of the variables have been established.

It was demonstrated that a two column parametric pump arranged back-to-back can minimize reservoir mixing (that normally occurs in a one column process), and thereby improve separation. It was further demonstrated that purification of a given solute(s) in a multicomponent system, and a true multi-

component split (normally achieved in multicomponent distillation) can be attained more efficiently with fewer cycles. The performance characteristics necessary to achieve high recoveries were established. Mathematical models for the depletion of a given solute(s) (where minimum mixing occurs) were derived by the method of characteristics based on the assumption of a pseudo binary system, consisting of one solute and the common solvent. The purification of solute(s) was significantly increased by decreasing the bottom product withdrawal rate.

The dilute product was found to be very sensitive to the number of cells (number of theoretical plates) used, while the enriched product was not affected. A cyclic process with longer columns could result in higher separability for some components, but may not do so for others. Separation factor and steady state enrichment of component A [o-xylene] were found to increase, while the steady state enrichment of component B [anisole] was found to decrease with increase in stage duration time above the optimum. Separability of the solutes increased with recycle ratio, with a maximum separation for recycle ratio equal to unity and minimum for recycle ratio equal to zero. The separation of solute(s) would increase with an increase in product withdrawal rate until the ratio of feed volume to void volume displacement is 0.2. Thereafter, solute separation decreases. The column became saturated and the separation capability dropped off sharply as the total solute concentrations reached 20 percent volume. The separation of solutes increased sharply as the

column displacement volume increased to approximately one void volume. Thereafter, solute separation decreased.

A comprehensive experimental program is needed to quantitatively verify the theoretical results of the staged sequence cyclic process. Particular emphasis should be paid to the heat transfer problems so as to be able to determine precisely the mode of operation of this process. Optimization of the various operating conditions should also be done. In cyclic processes, a great deal of time is usually expended to the determination of the sorbent and solvent suitable for the separation problem at hand. Sorbent properties critical for cyclic separations, especially those that give a substantial measurable solute equilibrium shift should be studied. A mixture of solvents should be avoided to prevent demixing normally found in liquid-solid chromatography; and the solvent should have low viscosity to ensure rapid mass transfer and thus adequate column efficiency. The solvent should be significantly less volatile than any solute thereby rendering recovery of solute via distillation practical without the necessity to employ substantial fractional distillation or to expend energy evaporating solvents.

A scale-up and a complete feasibility study should be done to determine the commercial application, if any, of the staged sequence cyclic process. Other forms of cyclic thermodynamic variables such as pH, electric field, ionic strength, concentration and magnetic field should be employed to determine the versatility of the process.

APPENDIX I
BREAKTHROUGH AND DESORPTION
EXPERIMENTAL DATA

TABLE 1

Runs 36, 38 and 39

Saturation: 5% v/v O-Xylene and 5% v/v Anisole in N-Heptane

Desorption: 100% N-Heptane

Feed: y_{01} = O-Xylene, y_{02} = Anisole

Time, Mins	70°C		45°C		10°C	
	y_1/y_{01}	y_2/y_{02}	y_1/y_{01}	y_2/y_{02}	y_1/y_{01}	y_2/y_{02}
2	1.0086	1.0271	1.0000	0.9893	1.0192	1.0156
4	1.0153	1.0353	0.0084	1.0002	0.9989	0.9977
6	1.0000	1.0095	1.0011	1.0000	1.0224	1.0227
8	0.9940	0.9991	1.0145	1.0036	1.0081	1.0062
10	0.9991	1.0000	1.0013	0.9926	1.0000	1.0000
12	1.0252	1.0233	1.0170	0.9949	0.9443	0.9640
14	0.9103	0.9539	0.8696	0.9422	0.8587	0.9320
16	0.6939	0.8625	0.5973	0.7994	0.8429	0.8122
18	0.4716	0.7650	0.3759	0.7005	0.4570	0.7140
20	0.2755	0.6774	0.2133	0.6209	0.3222	0.6344
22	0.1348	0.6121	0.1098	0.5766	0.2073	0.5704
24	0.0530	0.5732	0.0494	0.5434	0.1253	0.5223
26	0.0185	0.5526	0.0205	0.5193	0.0786	0.4967
28	0.0083	0.5617	0.0097	0.5050	0.0489	0.4722
30	0.0049	0.5369	0.0056	0.5074	0.0294	0.4580
32	0.0042	0.5512	0.0043	0.5013	0.0193	0.4393
34	0.0036	0.5179	0.0037	0.4778	0.0114	0.4268

TABLE 2

Runs 40, 41 and 42

Saturation: 5% v/v Toluene and 5% v/v Anisole in 1% v/v Isopropyl Alcohol and 89% v/v N-Heptane

Desorption: 1% v/v Isopropyl Alcohol and N-Heptane

Feed: y_{01} = O-Xylene, y_{02} = Anisole

Time, Mins	70°C		46°C		4°C	
	y_1/y_{01}	y_2/y_{02}	y_1/y_{01}	y_2/y_{02}	y_1/y_{01}	y_2/y_{02}
2	0.9934	0.9954	1.0006	0.9943	1.0072	0.9946
4	1.0054	0.9991	0.9974	0.9962	1.0024	0.9906
6	1.0119	1.0122	0.9869	0.9866	0.9965	0.9859
8	1.0000	1.0000	1.0000	1.0000	1.0031	0.9945
10	0.7707	0.9296	0.9712	0.9794	1.0000	1.0000
12	0.2148	0.7646	0.6338	0.8980	0.6416	0.8660
14	0.0253	0.6247	0.14627	0.6964	0.2297	0.6265
16	0.0066	0.4390	0.02271	0.4943	0.0814	0.4385
18	0.0042	0.3090	0.0062	0.3688	0.0289	0.2811
20	0.0034	0.2329	0.0039	0.2059	0.0117	0.1769
22	0.0026	0.1730	0.0027	0.1232	0.0058	0.1054
24	0.0023	0.1217	0.0022	0.0752	0.0036	0.0659
26	0.0021	0.0804	0.0021	0.0412	0.0028	0.0429
28	0.0021	0.0473	0.0016	0.0220	0.0024	0.0248
30	0.0008	0.0202	0.0011	0.01109	0.0017	0.0168
32	0.0007	0.0103	0.0099	0.0062	--	--

TABLE 3

Runs 43, 44 and 45

Saturation: 1% v/v O-Xylene and 1% v/v Anisole in Heptane

Desorption: N-Heptane

Feed: y_{01} = O-Xylene, y_{02} = Anisole

Time, Mins	85°C		60°C		30°C	
	y_1/y_{01}	y_2/y_{02}	y_1/y_{01}	y_2/y_{02}	y_1/y_{01}	y_2/y_{02}
1	1.0000	1.1700	1.0000	1.0944	1.0000	1.0000
3	1.0180	1.0650	1.0190	1.2257	1.0000	1.0000
5	1.1105	1.0130	0.9930	1.1163	1.0413	0.9890
7	1.1031	1.0360	1.0000	1.0944	1.0218	0.9012
9	1.0000	1.0000	1.0170	1.1382	1.0325	0.9293
11	0.8758	0.9718	0.9994	1.0000	1.0260	0.9494
13	0.7313	0.9686	0.9696	0.9708	0.9830	0.8793
15	0.7438	0.7348	0.9967	0.9341	0.8780	0.8796
17	0.7224	0.6743	0.9983	0.9159	0.7460	0.8753
19	0.5971	0.5348	0.9812	0.8648	0.6087	0.7213
21	0.3009	0.3457	0.9815	0.8466	0.4760	0.7145
23	0.1540	0.2541	0.8979	0.8131	0.3530	0.6792
25	0.0498	0.1823	0.6618	0.7282	0.2427	0.6517
27	0.0164	0.1453	0.6421	0.7125	0.1670	0.6345
29	--	0.0954	0.2579	0.6492	0.1111	0.6125
31	--	0.0512	0.1187	0.6201	0.0680	0.5930
33	--	0.0105	0.04455	0.5988	0.0280	0.5011

APPENDIX II
ONE-COLUMN PARAMETRIC PUMPING
EXPERIMENTAL DATA

TABLE 4

Run 5

Ref: L21

One Column--Semicontinuous

Mode: Top Feed

Conditions: Binary System Acetophenone-n-Heptane Solution y_0 Acetophenone = 2.5% v/v; Feed Abs. = 0.673

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.25$, $P_B = 0.125$, $\lambda = 246$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.805	1.196	0.507	0.753
2	0.669	0.994	0.361	0.536
3	0.703	1.044	0.153	0.227
4	0.717	1.065	0.042	0.062
5	0.738	1.096	0.036	0.053
6	0.750	1.114	0.023	0.034
7	0.752	1.117	0.018	0.026
8	0.830	1.233	0.018	0.026
9	0.891	1.323	0.018	0.026
10	0.896	1.331	0.024	0.035
11	0.879	1.306	0.023	0.034
12	0.900	1.333	0.014	0.020
13	0.888	1.319	0.015	0.022
14	0.918	1.364	0.011	0.016

TABLE 5

Run 6

Ref: L22

One Column--Semicontinuous

Mode: Top Feed

Conditions: Binary System Toluene-n-Heptane Solution y_0 Toluene = 2.5% v/v; Feed Abs. = .226

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.25$, $P_B = 0.125$, $\lambda = 263$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.228	1.008	0.012	0.053
2	0.219	0.9690	0.023	0.123
3	0.354	1.566	0.026	0.115
4	0.394	1.743	0.35	0.1548
5	0.365	1.615	0.047	0.207
6	0.467	2.066	0.029	0.128
7	0.457	2.022	0.026	0.115
8	0.460	2.035	0.016	0.0707
9	0.551	2.438	0.011	0.048
10	0.586	2.592	0.000	0.000
11	0.683	3.022	0.018	0.057
12	0.654	2.893	0.000	0.000
13	0.650	2.876	0.018	0.057
14	0.592	2.619	0.003	0.013

TABLE 6

Run 7

Ref: L23

One Column--Semicontinuous

Mode: Top Feed

Conditions: Binary System Toluene-n-Heptane Solution y_0 Toluene = 2.5% v/v; Feed Abs. = .226

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.1$, $P_B = 0.025$, $\lambda = 263$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

<u>Cycle No.</u>	<u>Top Product (Absorbance)</u>		<u>Bottom Product (Absorbance)</u>	
	<u>y_T</u>	<u>y_T/y_0</u>	<u>y_B</u>	<u>y_B/y_0</u>
1	0.282	1.247	0.213	0.942
2	0.227	1.004	0.276	1.221
3	0.273	1.207	0.211	0.933
4	0.350	1.548	0.225	0.9955
5	0.445	1.969	0.167	0.7389
6	0.480	2.123	0.110	0.4867
7	0.555	2.455	0.032	0.1415
8	0.498	2.203	0.023	0.1017
9	0.467	2.066	0.040	0.176
10	0.533	2.358	0.012	0.053
11	0.435	1.924	0.021	0.092
12	0.487	2.154	0.034	0.150
13	0.460	2.035	0.017	0.075
14	0.532	2.353	0.003	0.0132

TABLE 7

Run 8

Ref: L24

One Column--Semicontinuous

Mode: Top Feed

Conditions: Binary System Acetophenone-n-Heptane Solution y_0 Acetophenone = 2.5% v/v; Feed Abs. = 0.673

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.1$, $P_B = 0.025$, $\lambda = 246$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	<u>Top Product (Absorbance)</u>		<u>Bottom Product (Absorbance)</u>	
	<u>y_T</u>	<u>y_T/y_0</u>	<u>y_B</u>	<u>y_B/y_0</u>
1	0.536	0.796	0.403	0.600
2	0.550	0.817	0.214	0.317
3	0.650	0.965	0.230	0.341
4	0.674	1.001	0.182	0.270
5	0.727	1.080	0.105	0.156
6	0.758	1.126	--	--
7	0.786	1.167	0.044	0.065
8	0.757	1.124	0.040	0.060
9	0.682	1.013	0.028	0.041
10	0.751	1.115	0.023	0.035
11	0.679	1.008	0.006	0.008
12	1.049	1.558	0.141	0.210
13	0.671	0.997	0.097	0.145
14	0.606	0.900	0.000	0.000

TABLE 8

Run 9

Ref: L25

One Column--Semicontinuous

Mode: Top Feed

Conditions: Binary System Acetophenone-n-Heptane Solution y_0 Acetophenone = 2.5% v/v; Feed Abs. = 0.683

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.4$, $P_B = 0.025$, $\lambda = 246$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.593	0.868	0.651	0.953
2	0.607	0.888	0.154	0.225
3	0.796	1.165	0.180	0.263
4	0.770	1.127	0.112	0.165
5	0.954	1.396	0.232	0.339
6	0.847	1.240	0.091	0.133
7	0.893	1.307	0.085	0.125
8	1.123	1.644	0.092	0.135
9	0.926	1.355	0.225	0.329
10	1.009	1.477	0.078	0.115
11	1.082	1.584	0.105	0.153
12	0.980	1.434	0.192	0.281
13	1.176	1.721	0.096	0.142
14	1.012	0.1481	0.222	0.325

TABLE 9

Run 10

Ref: L23

One Column--Semicontinuous

Mode: Top Feed

Conditions: Binary System Toluene-n-Heptane Solution y_0 Toluene = 2.5% v/v; Feed Abs. = 0.239

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.4$, $P_B = 0.025$, $\lambda = 263$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.211	0.882	0.227	0.953
2	0.274	1.146	0.135	0.565
3	0.328	1.372	0.119	0.501
4	0.339	1.418	0.129	0.540
5	0.410	1.715	0.124	0.520
6	0.447	1.870	0.123	0.515
7	0.531	2.221	0.125	0.525
8	0.517	2.163	0.124	0.523
9	0.574	2.401	0.129	0.542
10	0.567	2.372	0.134	0.561
11	0.558	2.334	0.135	0.565
12	0.618	2.585	0.125	0.524
13	0.617	2.581	0.139	0.582
14	0.550	2.301	0.138	0.579

TABLE 10

Run 11

Ref: L26

One Column--Continuous

Mode: Top Feed

Conditions: Binary System Toluene-n-Heptane Solution y_0 Toluene = 2.5% v/v; Feed Abs. = 0.235

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.4$, $P_B = 0.025$, $\lambda = 263$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.219	0.932	0.190	0.808
2	0.278	1.183	0.119	0.506
3	0.334	1.421	0.107	0.455
4	0.360	1.532	0.082	0.348
5	0.406	1.727	0.082	0.348
6	0.426	1.812	0.117	0.493
7	0.432	1.838	0.106	0.451
8	0.506	2.153	0.108	0.459
9	0.483	2.055	0.154	0.655
10	0.547	2.327	0.194	0.825
11	0.419	1.782	0.091	0.387
12	0.464	0.974	0.119	0.506
13	0.434	1.846	0.159	0.676
14	0.426	1.813	0.107	0.455

TABLE 11

Run 12

Ref: L29

One Column--Continuous

Mode: Top Feed

Conditions: Binary System Acetophenone-n-Heptane Solution y_0 Acetophenone = 2.5% v/v; Feed Abs. = 0.589

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.4$, $P_B = 0.025$, $\lambda = 246$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.759	0.288	0.217	0.368
2	1.138	1.932	0.044	0.074
3	1.005	1.706	0.158	0.268
4	1.151	1.954	0.035	0.059
5	1.314	2.230	0.021	0.035
6	1.306	2.217	0.084	0.142
7	1.277	0.034	2.168	0.057
8	1.318	2.237	0.037	0.0628
9	1.375	2.334	0.065	0.110
10	1.334	2.264	0.063	0.106
11	1.201	2.039	0.071	0.120
12	1.392	2.363	0.051	0.086
13	1.338	2.271	0.100	0.169
14	1.174	1.993	0.133	0.225

TABLE 12

Run 13

Ref: L27

One Column--Continuous

Mode: Bottom Feed

Conditions: Binary System Toluene-n-Heptane Solution y_0 Toluene = 2.5% v/v; Feed Abs. = 0.235

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.4$, $P_B = 0.025$, $\lambda = 263$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.246	0.046	0.177	0.753
2	0.303	1.289	0.161	0.685
3	0.345	1.468	0.158	0.672
4	0.406	1.727	0.151	0.642
5	0.403	1.714	0.157	0.668
6	0.398	1.693	0.154	0.655
7	0.460	1.957	0.162	0.689
8	0.428	1.821	0.150	0.638
9	0.478	2.034	0.151	0.642
10	0.435	1.851	0.150	0.638
11	0.495	2.106	0.145	0.617
12	0.476	2.025	0.147	0.625
13	0.403	1.714	0.151	0.642
14	0.565	2.404	0.153	0.651

TABLE 13

Run 14

Ref: L28

One Column--Continuous

Mode: Bottom Feed

Conditions: Binary System Acetophenone-n-Heptane Solution y_0 Acetophenone = 2.5% v/v; Feed Abs. = 0.529

Half Cycle Time = 20 mins;

Displacement Volume = 40 cc

 $P_T + P_B = 0.4$, $P_B = 0.025$, $\lambda = 246$ $T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Top Product (Absorbance)		Bottom Product (Absorbance)	
	y_T	y_T/y_0	y_B	y_B/y_0
1	0.404	0.763	0.382	0.722
2	0.336	0.635	0.323	0.610
3	0.180	0.340	0.296	0.559
4	1.151	0.285	0.295	0.557
5	0.164	0.310	0.256	0.483
6	0.155	0.293	0.278	0.525
7	0.131	0.247	0.281	0.531
8	0.105	0.198	0.285	0.538
9	0.333	0.629	0.278	0.525
10	0.492	0.930	0.279	0.527
11	0.635	1.197	0.288	0.544
12	0.842	1.591	0.275	0.519
13	0.886	2.674	0.268	0.506
14	0.830	1.568	0.264	0.499

APPENDIX III**TWO-COLUMN PARAMETRIC PUMPING****EXPERIMENTAL DATA**

TABLE 14

Run #20

Two-Columns--Alternating Top Feed

Conditions: Ternary System--Toluene-Acetophenone-n-Heptane Solution

y_{01} (Toluene) = 5.0% v/v

y_{02} (Acetophenone) = 5.0% v/v

Half Cycle Time = 20 mins.

Displacement Volume = 40 cc

$P_T = 0.1$; $P_T + P_B = 0.400$

$T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

<u>Cycle No.</u>	<u>Feed cc</u>	<u>Top Product Recovery (%)</u>			<u>Bottom Product Recovery (%)</u>		
		<u>cc</u>	<u>y₁</u>	<u>y₂</u>	<u>cc</u>	<u>y₁</u>	<u>y₂</u>
1	16	4	74.120	25.880	12	43.420	56.580
2	16	4	87.640	12.360	12	40.710	59.290
3	16	4	96.550	3.450	12	39.740	60.260
4	16	4	97.830	2.1740	12	39.750	60.250
5	16	4	98.260	1.744	12	38.260	61.740
6	16	4	99.040	0.957	12	38.570	61.430
7	16	4	99.560	0.438	12	37.100	62.900
8	16	4	100.000	0.000	12	35.880	64.120
9	16	4	100.000	0.000	12	38.680	61.320
10	16	4	100.000	0.000	12	39.120	60.88

TABLE 15

Run #21

Two-Columns--Alternating Top Feed

Conditions: Ternary System--Toluene-Acetophenone-n-Heptane Solution

y_{01} (Toluene) = 5.0% v/v

y_{02} (Acetophenone) = 5.0% v/v

Half Cycle Time = 20 mins.

Displacement Volume = 40 cc

$P_T = 0.200$; $P_T + P_B = 0.400$

$T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Feed		Top Product Recovery (%)		Bottom Product Recovery (%)		
	cc	cc	y_1	y_2	cc	y_1	y_2
1	16	8	70.290	29.710	8	40.660	59.340
2	16	8	86.780	13.220	8	36.990	63.010
3	16	8	97.340	2.659	8	35.470	64.530
4	16	8	98.460	1.544	8	34.690	65.310
5	16	8	97.520	2.482	8	34.050	65.950
6	16	8	92.620	7.382	8	33.470	66.530
7	16	8	96.840	3.162	8	33.350	66.650
8	16	8	97.740	2.258	8	33.260	66.740
9	16	8	97.860	2.141	8	32.730	67.270
10	16	8	98.250	1.754	8	32.450	67.550

TABLE 16

Run #22

Two-Columns--Alternating Top Feed

Conditions: Ternary System--Toluene-Acetophenone-n-Heptane
Solution

y_{01} (Toluene) = 5.0% v/v

y_{02} (Acetophenone) = 5.0% v/v

Half Cycle Time = 20 mins.

Displacement Volume = 40 cc

$P_T = 0.300$; $P_T + P_B = 0.400$

$T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Feed		Top Product Recovery (%)		Bottom Product Recovery (%)		
	cc	cc	y_1	y_2	cc	y_1	y_2
1	16	12	63.310	36.690	4	44.560	55.440
2	16	12	75.190	24.810	4	41.030	58.970
3	16	12	75.720	24.280	4	39.250	60.750
4	16	12	80.930	19.070	4	38.440	61.560
5	16	12	73.980	26.02	4	36.640	63.360
6	16	12	75.430	24.57	4	35.440	64.560
7	16	12	71.160	28.84	4	35.110	64.890
8	16	12	67.150	32.85	4	34.760	65.240
9	16	12	66.440	33.56	4	33.110	66.890
10	16	12	66.090	33.91	4	33.320	66.680

TABLE 17

Run #23

Two-Columns--Alternating Top Feed

Conditions: Ternary System--Toluene-Acetophenone-n-Heptane Solution

y_{01} (Toluene) = 5.0% v/v

y_{02} (Acetophenone) = 5.0% v/v

Half Cycle Time = 20 mins.

Displacement Volume = 40 cc

$P_T = 0.1$; $P_T + P_B = 0.200$

$T_2 = 70^\circ\text{C}$; $T_1 = 25^\circ\text{C}$

Cycle No.	Feed cc	Top Product Recovery (%)			Bottom Product Recovery (%)		
		cc	y_1	y_2	cc	y_1	y_2
1	8	4	57.610	42.390	4	40.350	59.65
2	8	4	76.060	23.940	4	40.740	59.26
3	8	4	88.290	11.710	4	39.110	60.89
4	8	4	96.110	3.894	4	37.390	62.61
5	8	4	98.420	1.584	4	35.890	64.16
6	8	4	99.160	0.839	4	34.87	65.13
7	8	4	99.480	0.517	4	34.150	65.85
8	8	4	99.550	0.445	4	32.850	67.15
9	8	4	99.770	0.225	4	32.05	67.95
10	8	4	100.00	0.000	4	32.04	67.96

APPENDIX IV

ONE-COLUMN CYCLING ZONE

EXPERIMENTAL DATA

TABLE 18

Run #45

Conditions: Temperature Switching Time for
 $(T_1 = 25) = (T_2 = 60) = 10$ mins

$y_{01}(\text{O-Xylene}) = 1.0$ vol %;

$y_{02}(\text{Anisole}) = 1.0$ vol %

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y_1/y_{01}</u>	<u>y_2/y_{02}</u>
1	60	0.8879	1.2827
		0.9195	1.1507
		1.0367	1.197
		1.0885	1.1581
		1.227	1.217
		1.2534	1.1813
	25	1.3885	1.2612
		1.2879	1.0994
		1.2321	1.0153
		1.1482	0.9000
		1.0701	0.7197
		1.1954	0.68164
2	60	1.3580	0.6811
		1.5511	0.7250
		1.6517	0.7900
		1.6224	0.8339
	25	1.6224	0.9122
		1.4680	0.9058
		1.2212	0.8104
		1.1195	0.7445

TABLE 18 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
3	60	1.0597	0.6229
		1.1275	0.5933
		1.2856	0.6054
		1.5310	0.6800
		1.5316	0.7223
	25	1.5994	0.8027
		1.5356	0.8524
		1.3787	0.8614
		1.1683	0.8075
		1.0747	0.7720
4	60	0.9247	0.6197
		0.9643	0.5298
		1.1729	0.5674
		1.2471	0.5674
		1.2471	0.6393
	25	1.2321	0.6842
		1.2614	0.7371
		1.1477	0.7503
		0.9959	0.7160
		0.8183	0.6340
5	60	0.7649	0.5658
		0.7540	0.5060
		0.9051	0.5325
		1.0614	0.5616
		1.1614	0.6282

TABLE 18 (Cont'd.).

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
	25	1.1212	0.6292
		1.1212	0.6710
		1.0988	0.7123
		0.9568	0.6689
		0.8086	0.5912

TABLE 19

Run #46

Conditions: Temperature Switching Time for
(T₂ = 60) = (T₃ = 85) = 10 mins

y₀₁(Toluene) = 1.0 vol %;

y₀₂(Anisole) = 1.0 vol %

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
1	85	0.8339	1.3056
		0.8574	1.2421
		0.9224	1.2384
		1.0260	1.3516
	60	1.0511	1.5616
		1.1300	1.7392
		0.9270	1.6107
		0.9706	1.8677
		0.8385	1.6557
		0.84771	1.5864
2	85	0.8557	1.4727
		0.8419	1.3966
		0.9310	1.4865
		0.9873	1.6663
	60	1.0281	2.0100
		1.0695	2.1819
		0.9385	2.1041
		0.8908	2.1258
		0.8310	1.8947
		0.8402	1.7303

TABLE 19 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y1/y01</u>	<u>y2/y02</u>
3	85	0.8252	1.5039
		0.8396	1.4415
		0.9068	1.4764
		0.9994	1.6869
		1.0109	1.8979
	60	1.0568	2.0920
		0.9965	2.1274
		0.9413	2.0962
		0.8482	1.7990
		0.8327	1.5568

TABLE 20

Run #47

Conditions: **Temperature Switching Time for

($T_1 = 25$) = ($T_2 = 60$) = 10 mins

y_{01} (O-Xylene) = 1.0 vol %;

y_{02} (Anisole) = 1.0 vol %

*All runs are adjusted for temperature lag of 4 mins.

**Transients not included in data

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y_1/y_{01}</u>	<u>y_2/y_{02}</u>
3	60	0.8196	0.5217
		0.9848	0.5628
		1.0849	0.6149
		1.1496	0.7061
		1.1021	0.7075
	25	1.0667	0.7606
		1.0443	0.8275
		0.8759	0.7649
		0.6824	0.6125
		0.6407	0.4863
4	60	0.7179	0.4710
		0.9504	0.5231
		1.1063	0.5570
		1.0615	0.5604
		1.1131	0.6091

TABLE 20 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>		
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>	
5	25	1.0683	0.6488	
		0.9864	0.6813	
		0.8315	0.6430	
		0.6569	0.5069	
		0.6824	0.4424	
		0.7518	0.4295	
	60	0.9551	0.4696	
		1.1006	0.5193	
		1.1454	0.5914	
		1.0735	0.6220	
		25	0.9822	0.6407
			0.8524	0.6225
			0.6798	0.5274
			0.6736	0.4586
		0.7022	0.3927	

TABLE 21

Run #48

Conditions: **Temperature Switching Time for

($T_1 = 30$) = ($T_2 = 60$) = 10 mins

y_{01} (O-Xylene) = 1.0 vol %;

y_{02} (Anisole) = 1.0 vol %

*All runs are adjusted for temperature lag of 4 mins.

**Transients not included in data

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y_1/y_{01}</u>	<u>y_2/y_{02}</u>
3	30	0.6294	1.4900
		0.5617	1.0139
		--	--
		0.5429	0.6512
		0.5890	0.5857
		60	0.6190
	85	0.7181	0.5563
		0.8345	0.7056
		1.2484	1.4445
		0.7181	1.1071
		1.1423	1.8355
		0.9262	1.2450
		0.9361	1.4690
		1.0756	1.7916
1.0488	1.6613		

TABLE 21 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y1/y01</u>	<u>y2/y02</u>
4	30	1.2710	1.6001
		0.7407	0.8928
		0.6580	0.70139
		0.7327	0.5630
		1.5838	0.5563
	60	0.8722	0.4900
		0.9953	0.5588
		1.3081	1.4196
		0.9976	0.9430
		0.9079	0.9388
	85	1.1939	1.2142
		1.4053	1.8477
		1.3100	1.7351
		0.9934	1.2425
		0.8393	0.9633
5	30	0.7242	0.7123
		0.6777	0.5921
		0.7595	0.5440
		0.7421	0.4917
		0.7750	0.4555
	60	1.5622	0.5204
		0.9029	0.4968
		1.0230	0.6237
		0.9403	0.7507
		1.0230	0.9295

TABLE 21 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
	85	1.0436	0.8873
		1.2930	1.0906
		1.1916	1.2492
		1.7703	1.3839
		1.7703	1.3839
		1.2470	1.3171

TABLE 22

Run #49

Conditions: **Temperature Switching Time for

$(T_1 = 30) = (T_2 = 60) = (T_3 = 85) = 10$ mins

$y_{01}(\text{O-Xylene}) = 1.0$ vol %;

$y_{02}(\text{Anisole}) = 1.0$ vol %

*All runs are adjusted for temperature lag of 4 mins.

**Transients not included in data

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y_1/y_{01}</u>	<u>y_2/y_{02}</u>
3	85	0.8919	0.7853
		0.9887	0.8490
		1.0601	0.9266
		0.9689	1.2053
		0.9276	1.3471
		0.8562	1.2960
	30	0.8661	1.2741
		0.7618	1.1189
		0.6308	0.8283
		0.6641	0.6938
		0.7609	0.6284
		0.7736	0.5191
	60	0.7839	0.4458
		0.9422	0.4559
		1.0258	0.4690
		1.1329	0.4985
		1.2353	0.6191

TABLE 22 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y1/y01</u>	<u>y2/y02</u>
4	60	1.1146	0.6803
		1.085	0.7853
		1.0878	0.9110
		1.0427	0.9552
	85	0.9628	0.8696
		1.2475	1.1362
		1.1540	1.2328
		1.0878	1.6139
		0.9920	1.4774
		0.9835	1.5444
		1.0493	1.5554
		30	0.9065
0.7689	1.0868		
0.6796	0.8426		
0.6665	0.6402		
0.7346	0.5782		
0.8891	0.5394		
0.8806	0.4681		
60	0.9835		0.4660
	1.0831	0.5107	
	1.1136	0.6039	
	1.2198	0.7764	
	1.1423	0.8469	
		0.9798	0.8165

TABLE 22 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
5	85	0.9436	0.8485
		1.1808	1.0687
		1.0634	1.1540
		1.0474	1.3829
		0.9633	1.4192
		0.9671	1.4635
		0.8900	1.3007
	30	0.7829	1.1045
		0.6815	0.9139
		0.6458	0.7410
		0.6852	0.6296
		0.7299	0.5318
		0.8008	0.4803
		0.9041	0.4542
60	0.9906	0.4567	
	1.1737	0.5470	
	1.2790	0.6474	
	1.2094	0.8228	
	1.1390	0.8274	
	1.0925	0.8692	
	1.0230	0.8608	

TABLE 23

Run #50

Conditions: **Temperature Switching Time for
($T_1 = 30$) = ($T_2 = 60$) = ($T_3 = 85$) = 10 mins

y_{01} (O-Xylene) = 1.0 vol %;

y_{02} (Anisole) = 1.0 vol %

*All runs are adjusted for temperature lag of 4 mins.

**Transients not included in data

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y_1/y_{01}</u>	<u>y_2/y_{02}</u>
5	85	1.1496	1.2287
		1.2500	1.4414
		1.1708	1.5974
		1.2721	1.8183
		1.1970	1.6866
	30	0.9531	0.2926
		0.8397	1.0301
		0.8780	0.8911
		0.8346	0.6669
		0.8467	0.5274
	60	0.9430	0.5457
		1.0907	0.6171
		1.1265	0.7575
		1.0987	0.9853
		1.0025	1.0548

TABLE 23 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
6	85	1.1098	1.1674
		1.2177	1.2287
		1.3331	1.4126
		1.343	1.5988
		1.1607	1.4135
	30	1.0267	1.2532
		0.8598	0.9432
		0.8533	0.7868
		0.8744	0.6692
		0.9117	0.6010
	60	0.9294	0.5503
		0.908	0.5160
		1.163	0.6097
		1.2547	0.7032
		1.0539	0.8892
7	85	1.1144	1.0379
		1.2016	1.1125
		1.3407	1.3660
		1.3210	1.4748
		1.2157	1.3842
	30	0.9581	1.0969
		0.8382	0.8504
		0.8009	0.6619
		0.8351	0.5425
		0.8623	0.4720

TABLE 23 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
	60	0.9889	0.5114
		1.1370	0.5475
		1.1365	0.5887
		1.0987	0.7456
		0.9909	0.8664
8	85	1.0861	0.9766
		1.2031	1.0580
		1.2091	1.1628
		1.2580	1.3545
		1.2071	1.3101

TABLE 24

Run #51

Conditions: **Temperature Switching Time for

(T₁ = 30) = 20 mins

(T₂ = 60) = (T₃ = 85) = 14 mins

y₀₁(O-Xylene) = 1.0 vol %;

y₀₂(Anisole) = 1.0 vol %

*All runs are adjusted for temperature lag of 4 mins.

**Transients not included in data

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
3	85	0.9524	0.3595
		1.1960	0.4307
		1.2220	0.4635
		1.2910	0.5698
		1.2930	0.6206
		1.2470	0.6618
		1.1520	0.6444
		0.9276	0.5706
	30	0.7319	0.4527
		0.6786	0.3883
		0.6695	0.3395
		0.6796	0.3101
		0.6971	0.2648
		0.7109	0.2373
		0.7674	0.2291
		0.8398	0.2201
	0.9119	0.2001	

TABLE 24 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
	60	0.9863	0.1972
		0.1680	0.2181
		1.3140	0.2439
		1.3520	0.2622
		1.3980	0.2823
		1.4150	0.3064
		1.3660	0.3058
		1.3520	0.3360
		1.3600	0.3537
		1.4640	0.3784
4	85	1.4930	0.4167
		1.4980	0.4754
		1.3770	0.4992
		1.3730	0.5486
		1.3560	0.5875
		1.2600	0.5767
		1.0380	0.5027
		0.9163	0.4376
		0.8906	0.3825
		0.9050	0.3328
	30	0.9518	0.3017
		0.9897	0.2602
		0.8114	0.1886
		1.0540	0.2160

TABLE 24 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
	60	0.9863	0.1972
		0.1680	0.2181
		1.3140	0.2439
		1.3520	0.2622
		1.3980	0.2823
		1.4150	0.3064
		1.3660	0.3058
	60	1.0931	0.2090
		1.1740	0.2119
		1.3290	0.2386
		1.3840	0.2578
		1.3790	0.2965
		1.3240	0.3157
		1.2320	0.3244

TABLE 25

Run #52

Conditions: **Temperature Switching Time for

($T_1 = 30$) = 10 mins

($T_2 = 60$) = ($T_3 = 85$) = 14 mins

y_{01} (O-Xylene) = 1.0 vol %;

y_{02} (Anisole) = 1.0 vol %

*All runs are adjusted for temperature lag of 4 mins.

**Transients not included in data

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentrations</u>	
		<u>y_1/y_{01}</u>	<u>y_2/y_{02}</u>
3	85	0.8093	0.9570
		0.8815	1.4670
		0.8349	1.5980
		0.8252	1.6400
		0.8292	1.6540
		0.8462	1.6150
		0.7241	1.3960
	30	0.6218	1.0940
		0.6180	0.8587
		0.6185	0.6772
		0.6832	0.5901
		0.8704	0.7922
		0.8791	0.5976
	60	0.9895	0.7028
		1.0150	0.8688
		1.0090	1.0200

TABLE 25 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>		
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>	
4	60	0.9733	1.0760	
		0.9197	1.0480	
		0.9003	1.0070	
	85	0.9941	1.0250	
		1.0790	1.4090	
		1.0720	1.5880	
		0.9933	1.7410	
		0.9588	1.6740	
		0.9502	1.5930	
		0.8772	1.431	
		30	0.7061	1.1070
			0.6501	0.8511
			0.6563	0.6697
			0.7093	0.5612
			0.7576	0.4892
60	0.8195	0.4531		
	0.9690	0.5001		
	1.0810	0.6138		
	1.076	0.7462		
	1.0230	0.8680		
	0.9838	0.9600		
	0.9152	0.9552		

TABLE 25 (Cont'd.)

<u>Cycle No.</u>	<u>Temp. °C</u>	<u>Effluent Concentration</u>	
		<u>y₁/y₀₁</u>	<u>y₂/y₀₂</u>
	85	0.9030	0.9143
		0.9973	1.0050
		0.9777	1.1310
		0.9284	1.2580
		0.8799	1.2950
		0.8559	1.2670
		0.7904	1.1620

TABLE 26

Run #53

One-Column--Staged Sequence

Conditions: Ternary System--O-Xylene-Anisole-n-Heptane Solution

Recycle Ratio = 1.0

 $y_{01}(\text{O-Xylene}) = 10\% \text{ v/v}$ $y_{02}(\text{Anisole}) = 10\% \text{ v/v}$ Thermal Switching Period: $T_{30}=t_{60}=t_{85}=10 \text{ mins}$

Sample Size = 6cc

Cycle <u>No.</u>	<u>Product at 60°C</u>				<u>Product at 85°C</u>			
	<u>y_1/y_{01}</u>		<u>y_2/y_{02}</u>		<u>y_1/y_{01}</u>		<u>y_2/y_{02}</u>	
	<u>Exp.</u>	<u>Calc.</u>	<u>Exp.</u>	<u>Calc.</u>	<u>Exp.</u>	<u>Calc.</u>	<u>Exp.</u>	<u>Calc.</u>
1	1.23	1.26	0.75	0.77	0.98	0.92	1.33	1.36
2	1.28	1.26	0.78	0.73	0.98	1.01	1.32	1.26
3	1.25	1.23	0.68	0.64	0.99	1.06	1.30	1.25
4	1.23	1.20	0.65	0.60	0.96	1.02	1.29	1.27
5	1.23	1.96	0.63	0.60	0.95	1.01	1.28	1.23
6	1.20	1.18	0.60	0.59	0.94	0.99	1.27	1.23
7	1.15	1.17	0.59	0.58	0.96	0.98	1.23	1.20
8	1.14	1.16	0.59	0.58	0.98	0.97	1.18	1.19
9	1.19	1.16	0.58	0.57	0.98	0.97	1.21	1.17
10	1.18	1.55	0.55	0.57	0.94	0.96	1.90	1.16
11	1.20	1.50	0.59	0.56	0.93	0.95	1.20	1.14
12	1.19	1.46	0.58	0.56	0.92	0.95	1.75	1.13

TABLE 27

Run #54

One-Column--Staged Sequence

Conditions: Ternary System--O-Xylene-Anisole-n-Heptane Solution

Recycle Ratio = 0.0

 $y_{01}(\text{O-Xylene}) = 10\% \text{ v/v}$ $y_{02}(\text{Anisole}) = 10\% \text{ v/v}$ Thermal Switching Period: $T_{30}=t_{60}=t_{85}=10 \text{ mins}$

Sample Size = 6cc

Cycle No.	<u>Product at 60°C</u>				<u>Product at 85°C</u>			
	<u>y_1/y_{01}</u>		<u>y_2/y_{02}</u>		<u>y_1/y_{01}</u>		<u>y_2/y_{02}</u>	
	<u>Exp.</u>	<u>Calc.</u>	<u>Exp.</u>	<u>Calc.</u>	<u>Exp.</u>	<u>Calc.</u>	<u>Exp.</u>	<u>Calc.</u>
1	1.24	1.269	0.77	0.773	1.001	1.002	1.35	1.334
2	1.26	1.248	0.85	0.800	0.99	0.990	1.37	1.336
3	1.26	1.226	0.85	0.827	0.87	0.978	1.39	1.338
4	1.25	1.225	0.85	0.827	0.87	0.978	1.39	1.338
5	1.25	1.225	0.80	0.827	1.10	0.998	1.37	1.338
6	1.25	1.225	0.80	0.827	1.10	0.978	1.35	1.338
7	1.24	1.225	0.80	0.827	1.10	0.978	1.35	1.338
8	1.23	1.225	0.79	0.827	0.97	0.978	1.33	1.338
9	1.23	1.225	0.78	0.827	0.98	0.978	1.33	1.338
10	1.24	1.225	0.78	0.827	0.97	0.978	1.34	1.338
11	1.22	1.225	0.78	0.827	0.965	0.978	1.31	1.338
12	1.22	1.225	0.78	0.827	0.95	0.978	1.31	1.338

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AUGUST, 30TH, 1982

THIS PROGRAM CALCULATES THE CONCENTRATION PROFILES IN
THE SIMULATION OF A STAGED SEQUENCE CYCLIC PROCESS
USING THE METHCD CHARACTERISTICS AND A FOURTH ORDER
RUNGE KUTTA NUMERICAL ALGORITHM

N O M E N C L A T U R E

A = CROSS-SECTIONAL AREA , SQ.CM.
AMW = SURFACE AREA OF SOLID PER GRAM OF SOLID , GMMOLE/CC.
BMW = MOLECULAR WEIGHT OF O-XYLENE , CC./G.SOLID
CMW = MOLECULAR WEIGHT OF ANISOLE , GM./GMMOLE
DENS = DENSITY OF SILICA GEL , G-SOLID/CC.
DENB = DENSITY OF O-XYLENE , GMMOLE/CC.
DENC = DENSITY OF ANISOLE , GMMOLE/CC.
DB,DC = CONSTANTS IN MODIFIED LANGMUIR ISOTHERM ,
CC.PCRE/G.
DP = SOLID PARTICLE DIAMETER , CM.
ERR = TOLERANCE
H = HEIGHT OF THE COLUMN , CM.
N = NUMBER OF CYCLES
NNZ = NUMBER OF CELLS
NITER = NUMBER OF ITERATIONS
PB1,PB2,PB3 = TEMPERATURE DEPENDENT CONSTANTS IN MODIFIED
LANGMUIR ISOTHERM FOR O-XYLENE AT T1, T2 AND
T3 RESPECTIVELY
PC1,PC2,PC3 = TEMPERATURE DEPENDENT CONSTANTS IN MODIFIED
LANGMUIR ISOTHERM FOR ANISOLE AT T1, T2 AND
T3 RESPECTIVELY
QB1,QB2,QB3 = TEMPERATURE DEPENDENT CONSTANTS IN MODIFIED
LANGMUIR ISOTHERM FOR O-XYLENE AT T1, T2 AND
T3 RESPECTIVELY
QC1,QC2,QC3 = TEMPERATURE DEPENDENT CONSTANTS IN MODIFIED
LANGMUIR ISOTHERM FOR ANISOLE AT T1, T2 AND
T3 RESPECTIVELY
VISB1,VISB2,VISB3 = VISCOSITY OF O-XYLENE AT T1, T2, AND T3
VISC1,VISC2,VISC3 = VISCOSITY OF ANISOLE AT T1, T2, AND T3
RESPECTIVELY
TEMP1,TEMP2,TEMP3 = OPERATING TEMPERATURES DEGREES , K
TIME = STAGE DURATION TIME , MINS.
Q = COLUMN DISPLACEMENT VOLUME , CC.
VOID = COLUMN VOID VOLUME
VMB = MOLAR VOLUME OF O-XYLENE , CC./GMMOLE
VMC = MOLAR VOLUME OF ANISOLE , CC./GMMOLE
YA = INITIAL CONCENTRATION OF HEPTANE , GMMOLE/CC.
YBO = INITIAL CONCENTRATION OF O-XYLENE , GMMOLE/CC.
YCO = INITIAL CONCENTRATION OF ANISOLE , GMMOLE/CC.
YA1/YAO = NORMALIZED CONCENTRATION OF ANISOLE IN COLUMN 1
YB1/YBO = NORMALIZED CONCENTRATION OF ANISOLE IN COLUMN 2
YA2/YAO = NORMALIZED CONCENTRATION OF O-XYLENE IN COLUMN 2
YB2/YBO = NORMALIZED CONCENTRATION OF ANISOLE IN COLUMN 2

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C   YA3/YA0 = NORMALIZED CONCENTRATION OF O-XYLENE IN COLUMN 3
C   YB3/YB0 = NORMALIZED CONCENTRATION OF ANISOLE IN COLUMN 3
C
      DIMENSION YB1(100),YC1(100),YB2(100),YC2(100),
*YB3(100),YC3(100),XB1(100),XC1(100),XB2(100),XC2(100),
*XB3(100),XC3(100),YB12(100),YC12(100),YB13(100),
*YC13(100),YB11(100),YCB1(100),RAB1(100),RAC1(100),
*YB12(100),YCB2(100),RAB2(100),RAC2(100),XXB1(100),
*XXB2(100),XXB3(100),XXC1(100),XXC2(100),XXC3(100)
      DIMENSION YYB1(100),YYB2(100),YYB3(100),YYC1(100),
*YYC2(100),YYC3(100),YYBB1(100),YYCB1(100),YYBB3(100),
*YYBB2(100),YYCB2(100),YYBB3(100),YYCB3(100),RRAB1(100),
*RRAC1(100),RRAB2(100),RRAC2(100),RRAB3(100),RRAC3(100),
*YYYB1(100),YYYBB2(100),YYYBB3(100),YYYCB1(100),
*YYYCB2(100),YYYCB3(100),RRRAB1(100),RRRAC1(100)
      DIMENSION RRRAB2(100),RRRAB3(100),RRRAC2(100),
*RRRAC3(100),PHOT(100),PHOB(100),BETA(100),YCB3(100)
      DIMENSION RAB3(100),RAC3(100),SF1(50),SF2(50),SF3(50)
      COMMON VOID,DENS,VISA1,VISA2,VISA3,VISB1,VISB2,VISB3,
*VISC1,VISC2,VISC3,TEM1,TEM2,TEM3,PB1,PB2,PB3,
*PC1,PC2,PC3,QB1,QB2,QB3,QC1,QC2,QC3,V1,V2,V3,DT1,
*DT2,DT3,NITER,TIME,VMB,VMC,DB,DC,AMW,BMW,CMW,DP,AP,
*ERR,NZ,DENB,DENC
      READ 100,N,NNZ,NCASE,NITER,NR
100  FORMAT(5I6)
      READ 120,PB1,PB2,PB3,PC1,PC2,PC3
120  FORMAT(6F6.2)
      READ 130,QB1,QB2,QB3,QC1,QC2,QC3
130  FORMAT(6F6.2)
      READ 141,VISA1,VISA2,VISA3,VISB1,VISB2,VISC1,VISC2
      READ 90,VISA3,VISB3,VISC3
90   FORMAT(3F6.4)
141  FORMAT(6F6.4)
      READ 15,H,TIME,YA,YB0,YC0,Q
      READ 152,VT,VB,VOID,DENS,ERR,A
15   FORMAT(6F9.5)
152  FORMAT(6F9.5)
      READ 16,AP,DENB,DENC,DB,DC,DP
16   FORMAT(6F9.5)
      READ 17,TEM1,TEM2,TEM3,VMB,VMC
17   FORMAT(5F6.2)
      READ 18,AMW,BMW,CMW
18   FORMAT(3F6.2)
      DO 99I=1,NCASE
      READ 20,PHCT(I),PHOB(I),BETA(I)
99   CONTINUE
20   FORMAT(3F6.4)
30   FORMAT(2F6.4)
      DO 600 I=1,NCASE
2020 FORMAT('1')
11   FORMAT(/)
      PRINT 2020
      PRINT 3030
3030 FORMAT(9X,'N',8X,'NNZ',5X,'NCASE',5X,'NITER'//)
      PRINT 10,N,NNZ,NCASE,NITER,NR
      PRINT 11
      PRINT 3040
3040 FORMAT(10X,'PB1',10X,'PB2',10X,'PB3',10X,'PC1',

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*10X,'PC2',10X,'PC3'//)
  PRINT 12,PE1,PB2,PB3,PC1,PC2,PC3
  PRINT 11
  PRINT 3050
3050 FORMAT(10X,'QB1',10X,'QB2',10X,'QB3',10X,
*'QC1',10X,'QC2',10X,'QC3'//)
  PRINT 13,QE1,QE2,QE3,QC1,QC2,QC3
  PRINT 11
  PRINT 3060
3060 FORMAT(7X,'VISA1',7X,'VISA2',7X,'VISB1',7X,'VISB2',
*7X,'VISC1',7X,'VISC2')
  PRINT 14,VISA1,VISA2,VISB1,VISB2,VISC1,VISC2
  PRINT 3061
3061 FORMAT(7X,'VISA3',7X,'VISB3',7X,'VISC3')
  PRINT 9,VISA3,VISB3,VISC3
  PRINT 11
  PRINT 3070
3070 FORMAT(5X,'H',5X,'TIME',5X,'YA',5X,'YBO',5X,'YCO',
*5X,'Q',5X,'VT',5X,'VB')
  PRINT 15,H,TIME,YA,YBO,YCO,Q,VT,VB
  PRINT 11
  PRINT 3080
3080 FORMAT(7X,'VOID',7X,'DENS',7X,'ERR',7X,'A',//)
  PRINT 15,VOID,DENS,ERR,A
  PRINT 11
  PRINT 3090
3090 FORMAT(10X,'AP',10X,'DENB',10X,'DENC',10X,'DB',
*10X,'DC',10X,'DP')
  PRINT 16,AP,DENB,DENC,DB,DC,DP
  PRINT 11
  PRINT 4010
4010 FORMAT(10X,'TEM1',10X,'TEM2',10X,
*'TEM3',10X,'VMB',10X,'VMC'//)
  PRINT 17,TEM1,TEM2,TEM3,VMB,VMC
  PRINT 11
  PRINT 4020
4020 FORMAT(10X,'AMW',10X,'BMW',10X,'CMW'//)
  PRINT 18,AMW,BMW,CMW
  PRINT 11
  PRINT 7070
7070 FORMAT(6X,'PHOT',6X,'PHOB',6X,'BETA'//)
  PRINT 20,PHOT(I),PHOB(I),BETA(I)
  PRINT 2020
  V1=(BETA(I)+PHOT(I)+PHOB(I))*Q/(A*VOID*TIME)
  V2=(BETA(I)+PHOT(I)+PHOB(I))*Q/(A*VOID*TIME)
  V3=(BETA(I)+PHOT(I))*Q/(A*VOID*TIME)
  DT1=H/(NNZ*V1)
  DT2=H/(NNZ*V2)
  DT3=H/(NNZ*V3)
  PRINT 111,V1,V2,V3,DT1,DT2,DT3
111 FORMAT(15X,'V1=',F10.5,5X,'V2=',F10.5,5X,
*'V3=',F10.5,5X,'DT1=',F10.5,5X,'DT2=',F10.5,5X,
*'DT3=',F10.5)
  NZ=NNZ+1
  YBP1=YB0
  YCP1=YC0
  YBP2=YB0
  YCP2=YC0

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YBP3=YB0
YCP3=YC0
DO 21 J=1,NZ
YB1(J)=YB0
YC1(J)=YC0
21 CALL EQYTOX(PB3,PC3,QB3,QC3,DB,DC,YB1(J),YC1(J),
*DENB,DENC,XB1(J),XC1(J))
DO 22 J=1,NZ
YB2(J)=YB0
YC2(J)=YC0
22 CALL EQYTOX(PB3,PC3,QB3,QC3,DB,DC,YB2(J),YC2(J),
*DENB,DENC,XB2(J),XC2(J))
DO 23 J=1,NZ
YB3(J)=YB0
YC3(J)=YC0
23 CALL EQYTOX(PB3,PC3,QB3,QC3,DB,DC,YB3(J),YC3(J),
*DENB,DENC,XB3(J),XC3(J))
M=1
IF (M-1) 31,31,32
31 YBP1=YB0
YCP1=YC0
GO TO 33
32 YBP1=YYBB3(M-1)
YCP1=YYCB3(M-1)
IF (NR.EQ.0)YBP1=YB0*(1.-BETA(I))+YYBB3(M-1)*BETA(I)
IF (NR.EQ.0)YCP1=YC0*(1.-BETA(I))+YYCB3(M-1)*BETA(I)
33 YBIN=((PHOT(I)+PHOB(I))*YB0+YBP1*BETA(I))
*/(PHOT(I)+PHOB(I)+BETA(I))
YCIN=((PHOT(I)+PHOB(I))*YC0+YCP1*BETA(I))
*/(PHOT(I)+PHOB(I)+BETA(I))
IND=1
TEMP=TEM1
PRINT 222,M,YBP1,YCP1,YBIN,YCIN
222 FORMAT(5X,'M=',I5,5X,'YBP1=',E20.5,5X,'YCP1=',E20.5,
*5X,'YBIN=',E20.5,5X,'YCIN=',E20.5///)
CALL CONC(IND,XB1,XC1,YB1,YC1,YBIN,YCIN,XXB1,XXC1,
*YB1,YYC1,YBB,YCB,M,YA,YB0,YC0)
YBB1(M)=YBB
YCB1(M)=YCB
IF (M.EQ.1)GO TO 801
RAB1(M)=(YBB1(M)+YBB1(M-1))/(2.*YB0)
RAC1(M)=(YCB1(M)+YCB1(M-1))/(2.*YC0)
GO TO 802
801 RAB1(M)=YBB1(M)/YB0
RAC1(M)=YCB1(M)/YC0
802 PRINT 800,M,TEMP,YBB1(M),YCB1(M),RAB1(M),RAC1(M)
800 FORMAT(3X,'M=',I10,5X,'TEMP=',F6.2,5X,'YBB1=',
*E15.5,5X,'YCB1=',E15.5,5X,'RAB1=',E15.5,5X,'RAC1=',
*E15.5///)
IND=2
TEMP=TEM2
YBIN=YB1(NZ)
YCIN=YC1(NZ)
CALL CONC(IND,XB2,XC2,YB2,YC2,YBIN,YCIN,XXB2,
*XXC2,YYB2,YYC2,YBB,YCB,M,YA,YB0,YC0)
YBB2(M)=YBB
YCB2(M)=YCB
IF (M.EQ.1)GO TO 806

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      RAB2(M)=(YBB2(M)+YBB2(M-1))/(2.*YB0)
      RAC2(M)=(YCB2(M)+YCB2(M-1))/(2.*YCO)
      GO TO 807
506  RAB2(M)=YBB2(M)/YB0
      RAC2(M)=YCB2(M)/YCO
807  PRINT 805,M,TEMP,YBB2(M),YCB2(M),RAB2(M),RAC2(M)
805  FORMAT(3X,'M=',I10,5X,'TEMP=',F6.2,5X,'YBB2=',
*E15.5,5X,'YCB2=',E15.5,5X,'RAB2=',E15.5,5X,
*'RAC2=',E15.5///)
      IND=3
      TEMP=TEM3
      YBIN=YB2(NZ)
      YCIN=YC2(NZ)
      CALL CONC(IND,XB3,XC3,YB3,YC3,YBIN,YCIN,XXB3,XXC3,
*YYB3,YYC3,YBB,YCB,M,YA,YB0,YCO)
      YBB3(M)=YBB
      YCB3(M)=YCB
      IF(M.EQ.1)GO TO 808
      RAB3(M)=(YBB3(M)+YBB3(M-1))/(2.*YB0)
      RAC3(M)=(YCB3(M)+YCB3(M-1))/(2.*YCO)
      GO TO 809
808  RAB3(M)=YBB3(M)/YB0
      RAC3(M)=YCB3(M)/YCO
809  PRINT 810,M,TEMP,YBB3(M),YCB3(M),RAB3(M),RAC3(M)
*810  FORMAT(3X,'M=',I10,5X,'TEMP=',F6.2,5X,
*'YBB3=',E15.5,5X,'YCB3=',E15.5,5X,'RAB3=',E15.5,5X,
*/, 'RAC3=',E15.5///)
      IF(M-1)51,51,52
51  YYBP1=YB0
      YYCP1=YCO
      GO TO 53
52  YYBP1=YB3(NZ)
      YYCP1=YC3(NZ)
      IF(NR.EQ.0)YYBP1=YB0*(1.-BETA(I))+YB3(NZ)*BETA(I)
      IF(NR.EQ.0)YYCP1=YCO*(1.-BETA(I))+YC3(NZ)*BETA(I)
53  YYBIN=YYBP1
      YYCIN=YYCP1
      PRINT 333,M,YYBIN,YYCIN
333  FORMAT(5X,'M=',I10,5X,'YYBIN=',E15.5,5X,
*'YYCIN=',E15.5///)
      DO 60 L=1,NZ
      XB1(L)=XXB1(L)
      XC1(L)=XXC1(L)
      XB2(L)=XXB2(L)
      XC2(L)=XXC2(L)
      XB3(L)=XXB3(L)
      XC3(L)=XXC3(L)
      YB1(L)=YYB1(L)
      YC1(L)=YYC1(L)
      YB2(L)=YYB2(L)
      YC2(L)=YYC2(L)
      YB3(L)=YYB3(L)
60  YC3(L)=YYC3(L)
      IND=2
      TEMP=TEM2
      CALL CONC(IND,XB1,XC1,YB1,YC1,YYBIN,YYCIN,XXB1,
*XXC1,YYB1,YYC1,YBB,YCB,M,YA,YB0,YCO)
      YBB1(M)=YBB

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YYCB1(M)=YCB
IF(M.EQ.1)GO TO 811
RRAB1(M)=(YYBB1(M)+YYBB1(M-1))/(2.*YB0)
RRAC1(M)=(YYCB1(M)+YYCB1(M-1))/(2.*YCO)
GO TO 812
811 RRAB1(M)=YYBB1(M)/YB0
RRAC1(M)=YYCB1(M)/YCO
812 PRINT 74,M,TEMP,YYBB1(M),YYCB1(M),RRAB1(M),
*RRAC1(M)
74 FORMAT(3X,'M=',I10,5X,'TEMP=',F6.2,5X,'YYBB1=',
*E15.5,5X,'YYCB1=',E15.5,5X,'RRAB1=',E15.5,
*/,5X,'RRAC1=',E15.5///)
IND=3
TEMP=TEM3
YYBIN=YB1(NZ)
YYCIN=YC1(NZ)
CALL CONC(IND, XB2, XC2, YB2, YC2, YYBIN, YYCIN, XXB2,
*XXC2, YYB2, YYC2, YBB, YCB, M, YA, YB0, YCO)
YYBB2(M)=YBB
YYCB2(M)=YCB
IF(M.EQ.1)GO TO 813
RRAB2(M)=(YYBB2(M)+YYBB2(M-1))/(2.*YB0)
RRAC2(M)=(YYCB2(M)+YYCB2(M-1))/(2.*YCO)
GO TO 814
813 RRAB2(M)=YYBB2(M)/YB0
RRAC2(M)=YYCB2(M)/YCO
814 PRINT 72,M,TEMP,YYBB2(M),YYCB2(M),RRAB2(M),
*RRAC2(M)
72 FORMAT(3X,'M=',I10,5X,'TEMP=',F6.2,5X,
*'YYBB2=',E15.5,5X,'YYCB2=',E15.5,5X,
*'RRAB2=',E15.5,5X,/, 'RRAC2=',E15.5///)
IND=1
TEMP=TEM1
YYBIN=(YB2(NZ)*BETA(I)+(PHOT(I)+PHOB(I))*YB0)/
*(BETA(I)+PHOT(I)+PHOB(I))
YYCIN=(YC2(NZ)*BETA(I)+(PHOT(I)+PHOB(I))*YCO)/
*(BETA(I)+PHOT(I)+PHOB(I))
CALL CONC(IND, XB3, XC3, YB3, YC3, YYBIN, YYCIN,
*XXB3, XXC3, YYB3, YYC3, YBB, YCB, M, YA, YB0, YCO)
YYBB3(M)=YBB
YYCB3(M)=YCB
IF(M.EQ.1)GO TO 815
RRAB3(M)=(YYBB3(M)+YYBB3(M-1))/(2.*YB0)
RRAC3(M)=(YYCB3(M)+YYCB3(M-1))/(2.*YCO)
GO TO 816
815 RRAB3(M)=YYBB3(M)/YB0
RRAC3(M)=YYCB3(M)/YCO
816 PRINT 73,M,TEMP,YYBB3(M),YYCB3(M),RRAB3(M),RRAC3(M)
73 FORMAT(3X,'M=',I10,5X,'TEMP=',F6.2,5X,'YYBB3=',
*E15.5,5X,'YYCB3=',E15.5,5X,'RRAB3=',E15.5,5X,
*/, 'RRAC3=',E15.5///)
DO 75 L=1,NZ
XB1(L)=XXB1(L)
XC1(L)=XXC1(L)
XB2(L)=XXB2(L)
XC2(L)=XXC2(L)
XB3(L)=XXB3(L)
XC3(L)=XXC3(L)

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YB1(L)=YYB1(L)
YC1(L)=YYC1(L)
YB2(L)=YYB2(L)
YC2(L)=YYC2(L)
YB3(L)=YYB3(L)
75 YC3(L)=YYC3(L)
   IF (M-1) 76,76,77
76  YY YEP1=YB0
   YY YCP1=YC0
   GO TO 78
77  YY YBP1=YB3(NZ)
   YY YCP1=YC3(NZ)
   IF (NR.EQ.0)YY YBP1=YB0*(1.-BETA(I))+YB3(NZ)*BETA(I)
   IF (NR.EQ.0)YY YCP1=YC0*(1.-BETA(I))+YC3(NZ)*BETA(I)
78  YY YBIN=YY YEP1
   YY YCIN=YY YCP1
   IND=3
   TEMP=TEM3
   CALL CONC(IND, XB1, XC1, YB1, YC1, YY YBIN, YY YCIN,
 *XXB1, XXC1, YYB1, YYC1, YBB, YCB, M, YA, YB0, YC0)
   YY YBB1(M)=YBB
   YY YCB1(M)=YCB
   IF (M.EQ.1)GO TO 817
   RRRAB1(M)=(YY YBB1(M)+YY YBB1(M-1))/(2.*YB0)
   RRRAC1(M)=(YY YCB1(M)+YY YCB1(M-1))/(2.*YC0)
   GO TO 818
817 RRRAB1(M)=YY YBB1(M)/YB0
   RRRAC1(M)=YY YCB1(M)/YC0
818 PRINT 81, M, TEMP, YY YBB1(M), YY YCB1(M), RRRAB1(M),
 *RRRAC1(M)
81  FORMAT(3X, 'M=', I10, 5X, 'TEMP=', F6.2, 5X,
 *'YY YBB1=', E15.5, 5X, 'YY YCB1=', E15.5, 5X, 'RRRAB1=', E15.5,
 *5X, '/', 'RRRAC1=', E15.5//)
   IND=1
   TEMP=TEM1
   YY YBIN=(YB1(NZ)*BETA(I)+(PHOT(I)+PHOB(I))*YB0)/
 *(BETA(I)+PHOT(I)+PHOB(I))
   YY YCIN=(YC1(NZ)*BETA(I)+(PHOT(I)+PHOB(I))*YC0)/
 *(BETA(I)+PHOT(I)+PHOB(I))
   CALL CONC(IND, XB2, XC2, YB2, YC2, YY YBIN, YY YCIN,
 *XXB2, XXC2, YYB2, YYC2, YBB, YCB, M, YA, YB0, YC0)
   YY YBB2(M)=YBB
   YY YCB2(M)=YCB
   IF (M.EQ.1)GO TO 819
   RRRAB2(M)=(YY YBB2(M)+YY YBB2(M-1))/(2.*YB0)
   RRRAC2(M)=(YY YCB2(M)+YY YCB2(M-1))/(2.*YC0)
   GO TO 820
819 RRRAB2(M)=YY YBB2(M)/YB0
   RRRAC2(M)=YY YCB2(M)/YC0
820 PRINT 82, M, TEMP, YY YBB2(M), YY YCB2(M), RRRAB2(M),
 *RRRAC2(M)
82  FORMAT(3X, 'M=', I10, 5X, 'TEMP=', F6.2, 5X, 'YY YBB2=',
 *E15.5, 5X, 'YY YCB2=', E15.5, 5X, 'RRRAB2=', E15.5, 5X,
 */, 'RRRAC2=', E15.5//)
   IND=2
   TEMP=TEM2
   YY YBIN=YB2(NZ)
   YY YCIN=YC2(NZ)

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CALL CONC(IND, XB3, XC3, YB3, YC3, YYYB1N, YYYCIN,
*XB3, XC3, YB3, YC3, YBB, YCB, M, YA, YB0, YC0)
  YYYBB3(M) = YBB
  YYYCB3(M) = YCB
  IF (M.EQ.1) GO TO 821
  RRRAB3(M) = (YYYBB3(M) + YYYBB3(M-1)) / (2.*YB0)
  RRRAC3(M) = (YYYCB3(M) + YYYCB3(M-1)) / (2.*YC0)
  GO TO 822
821 RRRAB3(M) = YYYBB3(M) / YB0
  RRRAC3(M) = YYYCB3(M) / YC0
822 PRINT 83, M, TEMP, YYYBB3(M), YYYCB3(M), RRRAB3(M),
*RRRAC3(M)
83  FORMAT(3X, 'M=', I10, 5X, 'TEMP=', F6.2, 5X,
*'YYYBB3=', E15.5, 5X, 'YYYCB3=', E15.5, 5X,
*'RRRAB3=', E15.5, 5X, '/', 'RRRAC3=', E15.5//)
  DO 84 L=1, NZ
  XB1(L) = XB3(L)
  XC1(L) = XC3(L)
  XB2(L) = XB3(L)
  XC2(L) = XC3(L)
  XB3(L) = XB3(L)
  XC3(L) = XC3(L)
  YB1(L) = YB3(L)
  YC1(L) = YC3(L)
  YB2(L) = YB3(L)
  YC2(L) = YC3(L)
  YB3(L) = YB3(L)
84  YC3(L) = YC3(L)
  IF (M-N) 50, 500, 500
50  M=M+1
  GO TO 32
500 DO 501 M=1, N
  SF1(M) = RAB2(M) * RAC3(M) / (RAC2(M) * RAB3(M))
  SF2(M) = RRAB1(M) * RRAC2(M) / (RRAC1(M) * RRAB2(M))
501 SF3(M) = RRRAB3(M) * RRRAC1(M) / (RRRAC3(M) * RRRAB1(M))
  PRINT 510, (M, YBB1(M), YCB1(M), YBB2(M), YCB2(M),
*YBB3(M), YCB3(M), M=1, N)
510 FORMAT(' ', 3X, 'M', 5X, 'YBB1', 5X, 'YCB1',
*5X, 'YBB2', 5X, 'YCB2', 5X, 'YBB3', 5X, 'YCB3'//
*(5X, I5, 6E10.5))
  PRINT 511, (M, YYYBB1(M), YYYCB1(M), YYYBB2(M), YYYCB2(M),
*YYYBB3(M), YYYCB3(M), M=1, N)
511 FORMAT(' ', 3X, 'M', 5X, 'YYYBB1', 5X, 'YYYCB1', 5X,
*'YYYBB2', 5X, 'YYYCB2', 5X, 'YYYBB3', 5X, 'YYYCB3'//
*(5X, I5, 6E10.5))
  PRINT 512, (M, YYYBB1(M), YYYCB1(M), YYYBB2(M), YYYCB2(M),
*YYYBB3(M), YYYCB3(M), M=1, N)
512 FORMAT(' ', 3X, 'M', 5X, 'YYYBB1', 5X, 'YYYCB1', 5X,
*'YYYBB2', 5X, 'YYYCB2', 5X, 'YYYBB3', 5X,
*'YYYCB3'// (5X, I5, 6E10.5))
  PRINT 522, NNZ, H, TIME
  PRINT 523, PHOT(I), PHOB(I), BETA(I)
522 FORMAT(' ', 7X, 'NNZ=', I10, 2X, 'H=', F10.5, 2X, 'TIME=', F10.5)
523 FORMAT(7X, 'PHOT=', F10.5, 2X, 'PHOB=', F10.5, 2X,
*'BETA=', F10.5)
  PRINT 524, YB0, YC0, Q
524 FORMAT(7X, 'YB0=', F10.5, 2X, 'YC0=', F10.5, 2X, 'Q=', F10.5)
  PRINT 516

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516 FORMAT(15X,'CONCENTRATION TRANSIENTS IN STAGE 1')
PRINT 519
519 FORMAT(17X,'T1',16X,'T2',16X,'T3'/)
PRINT 513, (M,RAB1(M),RAC1(M),RAB2(M),RAC2(M),
* RAB3(M),RAC3(M),SF1(M),M=1,N)
513 FORMAT(7X,'M',2X,'YA1/YA0',2X,'YB1/YB0',2X,'YA2/YA0',
* 2X,'YB2/YB0',2X,'YA3/YA0',2X,
* 'YB3/YB0',2X,'SFACTOR'/(3X,15,7(2X,F7.5)))
PRINT 517
517 FORMAT(/,15X,'CONCENTRATION TRANSIENTS IN STAGE 2')
PRINT 520
520 FORMAT(17X,'T2',16X,'T3',16X,'T1'/)
PRINT 514, (M,RRAB1(M),RRAC1(M),RRAB2(M),RRAC2(M),
* RRAB3(M),RRAC3(M),SF2(M),M=1,N)
514 FORMAT(7X,'M',2X,'YA1/YA0',2X,'YB1/YB0',2X,'YA2/YA0',
* 2X,'YB2/YB0',2X,'YA3/YA0',2X,
* 'YB3/YB0',2X,'SFACTOR'/(3X,15,7(2X,F7.5)))
PRINT 518
518 FORMAT(/,15X,'CONCENTRATION TRANSIENTS IN STAGE 3')
PRINT 521
521 FORMAT(17X,'T3',16X,'T1',16X,'T2'/)
PRINT 515, (M,RRRAB1(M),RRRAC1(M),RRRAB2(M),RRRAC2(M),
* RRRAB3(M),RRRAC3(M),SF3(M),M=1,N)
515 FORMAT(7X,'M',2X,'YA1/YA0',2X,'YB1/YB0',2X,'YA2/YA0',
* 2X,'YB2/YB0',2X,'YA3/YA0',2X,
* 'YB3/YB0',2X,'SFACTOR'/(3X,15,7(2X,F7.5)))
600 CONTINUE
STOP
END

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SUBROUTINE CONC(IND,XB2,XC2,YB2,YC2,YBIN,YCIN,
*XXB,XXC,YYE,YYC,YYBAV,YYCAV,M,YA,YBO,YCO)
COMMON VOID,DENS,VISA1,VISA2,VISA3,VISB1,VISB2,
*VISB3,VISC1,VISC2,VISC3,TEM1,TEM2,TEM3,PB1,PB2,PB3,
*PC1,PC2,PC3,QB1,QB2,QB3,QC1,QC2,QC3,V1,V2,V3,DT1,DT2,
*DT3,NITER,TIME,VMB,VMC,DB,DC,AMW,BMW,CMW,DP,AP,ERR,NZ,
*DENB,DENC
DIMENSION XB2(100),XC2(100),YB2(100),YC2(100),XXB2(100),
*XXC(100),YYB(100),YYC(100),XBT(100),XCT(100),XXBS(100),
*XXCS(100),YYBS(100),YYCS(100),NTR(100),XXC2(100),
*YYB2(100),XXB(100),YYC2(100),YYB2EQ(100),YYC2EQ(100),
*YYB2ES(100),YYC2ES(100),RAYB(100),RAYC(100)
SUMB=YB2(NZ)
SUMC=YC2(NZ)
IF(IND.EQ.1)GO TO 20
IF(IND.EQ.2)GO TO 10
IF(IND.EQ.3)GO TO 37
10 VISA=VISA2
VISB=VISB2
VISC=VISC2
V=V2
PB=PB2
PC=PC2
QB=QB2
QC=QC2
DT=DT2

```

```

TEM=TEM 2
GO TO 30
20 VISA=VISA 1
VISB=VISB 1
VISC=VISC 1
V=V 1
PB=PB 1
PC=PC 1
QB=QB 1
QC=QC 1
DT=DT 1
TEM=TEM 1
GO TO 30
37 VISA=VISA 3
VISB=VISB 3
VISC=VISC 3
V=V 3
PB=PB 3
PC=PB 3
QB=QB 3
QC=QC 3
DT=DT 3
TEM=TEM 3
30 CNSTB=-(1.-VOID)*DENS/VOID
CNSTC=-(1.-VOID)*DENS/VOID
CNSTC=-(1.-VOID)*DENS/VOID
XBT(1)=XB2(1)
XCT(1)=XC2(1)
DO 22 L=1,NZ
XXB2(L)=XB2(L)
XXC2(L)=XC2(L)
YYB2(L)=YB2(L)
22 YYC2(L)=YC2(L)
K=1
155 CNK=K
TT=DT*CNK
YYB(1)=YBIN
YYC(1)=YCIN
CALL YSTAR(PB,PC,QB,QC,DB,DC,YBEQI,YCEQI,
*DENB,DENC,XXB2(1),XXC2(1))
CALL RUNGE(YYB2(1),YYC2(1),YBEQI,YCEQI,XXB2(1),XXC2(1),
*PB,PC,QB,QC,DB,DC,DENB,DENC,XB,XC,DT,YA,AMW,BMW,CMW,
*VISA,VISB,VISC,DP,VOID,VMB,VMC,V,AP,TEM)
XBT(K+1)=XB
XCT(K+1)=XC
XXB(1)=XBT(K+1)
XXC(1)=XCT(K+1)
RAYB(1)=YYB(1)/YBO
RAYC(1)=YYC(1)/YCO
I=2
C
85 ITER=1
NTR(1)=1
YYB2EQ(1)=YBEQI
YYC2EQ(1)=YCEQI
CALL CMSS(YA,YYB2(I-1),YYC2(I-1),AMW,BMW,CMW,VISA,VISB,
*VISC,DP,VOID,AP,VMB,VMC,CLB,CLC,V,TEM)
YYBS(I)=YYB2(I-1)+CNSTB*CLB+DT*(YYB2(I-1)-YYB2EQ(I-1))

```



```

YYC2(I) = YYC2(I-1) + CNSTC * CLC * DT * (YYC2(I-1) - YYC2EQ(I-1))
CALL YSTAR(PB, PC, QB, QC, DB, DC, YYB2EQ(I), YYC2EQ(I),
*DENB, DENC, XXB2(I), XXC2(I))
XXB2(I) = XXB2(I) + CLB * DT * (YYB2(I) - YYB2EQ(I))
XXC2(I) = XXC2(I) + CLC * DT * (YYC2(I) - YYC2EQ(I))
101 CALL YSTAR(PB, PC, QB, QC, DB, DC, YYB2ES(I), YYC2ES(I),
*DENB, DENC, XXB2(I), XXC2(I))
AQ1 = YYB2(I) + YYB2(I-1) - YYB2ES(I) - YYB2EQ(I-1)
AQ2 = AQ1 * (DT/2.) * CNSTB * CLB
YYB(I) = YYB2(I-1) + AQ2
BQ1 = YYC2(I) + YYC2(I-1) - YYC2ES(I) - YYC2EQ(I-1)
BQ2 = BQ1 * (DT/2.) * CNSTC * CLC
YYC(I) = YYC2(I-1) + BQ2
XXB(I) = XXB2(I) + (CLB * DT/2.) * (YYB2(I) + YYB2(I) - YYB2ES(I) -
*YYB2EQ(I))
XXC(I) = XXC2(I) + (CLC * DT/2.) * (YYC2(I) + YYC2(I) - YYC2ES(I) -
*YYC2EQ(I))
DEVYB = (YYB(I) - YYB2(I)) / YYB2(I)
DEVYC = (YYC(I) - YYC2(I)) / YYC2(I)
IF (ABS(DEVYB) - ERR) 50, 50, 60
50 IF (ABS(DEVYC) - ERR) 70, 70, 60
70 DEVXB = (XXB(I) - XXB2(I)) / XXB2(I)
DEVXC = (XXC(I) - XXC2(I)) / XXC2(I)
IF (ABS(DEVXB) - ERR) 80, 80, 60
80 IF (ABS(DEVXC) - ERR) 71, 71, 60
60 IF (ITER - NITER) 81, 71, 71
81 YYB(I) = YYB(I)
YYC(I) = YYC(I)
XXB(I) = XXB(I)
XXC(I) = XXC(I)
ITER = ITER + 1
GO TO 101
71 NTR(I) = ITER
RAYB(I) = YYB(I) / YB0
RAYC(I) = YYC(I) / YC0
IF (I - NZ) 82, 90, 90
82 I = I + 1
GO TO 85
90 SUMB = SUMB + YYB(NZ)
SUMC = SUMC + YYC(NZ)
IF (TT - TIME) 150, 200, 200
150 DO 151 L = 1, NZ
YYB2(L) = YYB(L)
YYC2(L) = YYC(L)
XXB2(L) = XXB(L)
151 XXC2(L) = XXC(L)
K = K + 1
GO TO 155
200 TOTK = K + 1
YYBAV = SUMB / TOTK
YYCAV = SUMC / TOTK
RETURN
END

```

C
C
C

SUBROUTINE RUNGE(YBI, YCI, YBEQI, YCEQI, XBI, XCI, PB, PC, QB, QC,
*DB, DC, DENB, DENC, XB, XC, TT, YA, AMW, BMW, CMW, VISA, VISB,

```

*VISC,DP,VOID,VMB,VMC,V,AP,TEM)
  CALL CMSS(YA,YBI,YCI,AMW,BMW,CMW,VISA,VISB,VISC,DP,
*VOID,AP,VMB,VMC,CLB,CLC,V,TEM)
  AKB1=CLB*(YBI-YBEQI)*TT
  AKC1=CLC*(YCI-YCEQI)*TT
  X2B=XBI+(AKB1/2.)
  X2C=XCI+(AKC1/2.)
  CALL YSTAR(PB,PC,QB,QC,DB,DC,YBEQ,YCEQ,DENB,DENC,
*X2B,X2C)
  AKB2=CLB*(YBI-YBEQ)*TT
  AKC2=CLC*(YCI-YCEQ)*TT
  X3B=XBI+(AKB2/2.)
  X3C=XCI+(AKC2/2.)
  CALL YSTAR(PB,PC,QB,QC,DB,DC,YBEQ,YCEQ,DENB,DENC,
*X3B,X3C)
  AKB3=CLB*(YBI-YBEQ)*TT
  AKC3=CLC*(YCI-YCEQ)*TT
  X4B=XBI+AKB3
  X4C=XCI+AKC3
  CALL YSTAR(PB,PC,QB,QC,DB,DC,YBEQ,YCEQ,DENB,DENC,
*X4B,X4C)
  AKB4=CLB*(YBI-YBEQ)*TT
  AKC4=CLC*(YCI-YCEQ)*TT
  DXB=(AKB1+2.*AKB2+2.*AKB3+AKB4)/6.
  DXC=(AKC1+2.*AKC2+2.*AKC3+AKC4)/6.
  XB=XBI+DXB
  XC=XCI+DXC
  RETURN
  END

```

C
C

```

SUBROUTINE CMSS(YA,YB,YC,AMW,BMW,CMW,VISA,VISB,
*VISC,DP,VOID,AP,VMB,VMC,CLB,CLC,V,TEM)
  ALPHB=0.005*EXP(-YB/0.00045)
  ZC=YC/0.0005
  ALPHC=0.005-0.00282*ZC+0.000925*ZC**2.-0.000103
**ZC**3.
  DEN=YA*AMW+YB*BMW+YC*CMW
  VIS=(VISA*YA+VISB*YB+VISC*YC)/(YA+YB+YC)
  FACT=(DP*V*VOID*DEN)/(VISC*(1.-VOID))
  FJB=ALPHB*(FACT**(-0.78))
  FJC=ALPHC*(FACT**(-0.78))
  DCONST=(7.4*10**(-8.0))*60.*(AMW**(0.5))
  DBA=DCONST*TEM/(VIS*VMB**(0.6))
  DCA=DCONST*TEM/(VIS*VMC**(0.6))
  CLB=AP*FJB*V*VOID*((DEN*DBA/VIS)**(2./3.))
  CLC=AP*FJC*V*VOID*((DEN*DCA/VIS)**(2./3.))
  RETURN
  END

```

C
C
C

```

SUBROUTINE EQYTOX(PB,PC,QB,QC,DB,DC,YB,YC,DENB,DENC,
*XB,XC)
  XB=PB*YB/(1.+QB*YB/DENB)+DB*YB
  XC=PC*YC/(1.+QC*YC/DENC)+DC*YC
  RETURN
  END

```

C
C
C

```
      SUBROUTINE YSTAR(PB,PC,QB,QC,DB,DC,YB,YC,DENB,DENC,  
*XB, XC)  
      CONSRB=(PB+DB)*DENB-QB*XB  
      YB=(-CONSRB+SQRT(CONSRB*CONSRB+4.*QB*DB*XB*DENB))  
*/(2.*QB*DB)  
      CONSRC=(PC+DC)*DENC-QC*XC  
      YC=(-CONSRC+SQRT(CONSRC*CONSRC+4.*QC*DC*XC*DENC))  
*/(2.*QC*DC)  
      RETURN  
      EN
```

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THIS PROGRAM PREDICTS THE RESPONSE OF A PULSE & STEP INPUT IN
 A PACKED BED

N O M E N C L A T U R E

Z=LENGTH OF COLUMN
 A=INTERFACIAL AREA PER UNIT VOLUME
 KX=INTERFACIAL MASS TRANSFER COEFFICIENT
 KM=EQUILIBRIUM CONSTANT
 DIMENSION AK(25),SIGMA(505),
 *XSIGMA(505),TSUM(505),XOUT(505),SSUM(505),
 *TPRIME(505),REALT(505),TTAU(505),
 *SSIGMA(505),SSSUM(505),XXOUT(505),TTPRIM(505),
 *RREALT(505),TTAUP(505),TSSUM(505),XXSIGM(505)
 REAL KX,KM,K2
 READ(5,48)N
 48 FORMAT(I2)
 NN=N+1
 DO 506 KK=1,NN
 READ(5,49)A,KX,KM
 49 FORMAT(F6.1,F7.5,F5.3)
 AREA=0.7853982
 Z=5.
 VOID=0.38
 VEL=1.00
 YF=1.0
 TAU=1.
 TAU=2.
 PT=TAUP-TAU
 DPT=PT/500.
 SI=(Z*AREA*A*KX)/VEL
 TP=(1.-VOID)/(KM*KX*A)
 RT=Z*(VOID*AREA*YF/VEL)
 DT=TAU/500.
 TPRIME(1)=0.0
 DO 50 I=2,501
 TPRIME(I)=DT*(I-1)*TP
 50 CONTINUE
 DO 55 I=1,501
 REALT(I)=TPRIME(I)+RT
 55 CONTINUE
 TTAU(1)=0.0
 DO 53 I=2,501
 TTAU(I)=(I-1)*DT
 53 CONTINUE

TTPRIM(1)=TPRIME(501)

```

DO 505 I=2,501
TTPRIM(I)=DPT*(I-1)*TP+TTPRIM(1)
505 CONTINUE
C
C
C
DO 550 I=1,501
RRALP(I)=ITPRIM(I)+RT
550 CONTINUE
C
C
C
TTAUP(1)=TTAU(501)
DO 530 I=2,501
TTALP(I)=(I-1)*DPT+TTAUP(1)
530 CONTINUE
C
C
C
C
C
C
C
COMPUTE FACTRIALS
C
C
C
AK(1)=1.0
DO 44 I=2,20
AK(I)=AK(I-1)*I
44 CONTINUE
C
C
C
C
C
C
COMPUTE ARGUMENT OF BESSEL FUNCTION
C
C
C
SIGMA(1)=0.0
SSUM(1)=1.0
TSUM(1)=0.0
DO 33 I=2,501
SIGMA(I)=DT*(I-1)
XX1=SIGMA(I)
X1=SQRT(4.*SI*XX1)
XSIGMA(I)=X1
C
C
C
C
C
COMPUTE SUM IN BESSEL FUNCTION
C
C
C
SUM=1.0
DO 333 II=1,20
X=(XSIGMA(I)/2.)*2.*II
SUM=SUM+(X/(AK(II))*2.)
333 CONTINUE
C
C
C
EXX=SIGMA(I)+SI
SSUM1=SUM*EXP(-EXX)
SSUM(I)=SSUM1
TSUM(I)=TSUM(I-1)+DT*(SSUM(I)+SSUM(I-1))/2.
33 CONTINUE
C

```

```

C
  AASUM=1.0
  DO 11 I=1,20
  SUM1=SQRT(4.*SI*TAU)/2.
  ASUM=SUM1**2.*I
  AASUM=(ASUM/(AK(I)**2.))+AASUM
11 CONTINUE
  XX=AASUM*EXP(-SI-TAU)
C
C
  DO 111 I=1,501
  XOUT(I)=XX+TSUM(I)
111 CONTINUE
C
  SSIGMA(1)=C.C
  SSSUM(1)=1.0
  TSSUM(1)=0.0
  DO 34 I=2,501
  SSIGMA(I)=DPT*(I-1)
  XX2=SSIGMA(I)
  X2=SQRT(4.*SI*XX2)
  XXSIGM(I)=X2
C
C
C
  SUM2=1.0
  DO 334 II=1,20
  XX=(XXSIGM(II)/2.)*2.*II
  SUM2=SUM2+(XX/(AK(II)**2.))
334 CONTINUE
  EEX=SSIGMA(I)+SI
  SSUM2=SUM2*EXP(-EEX)
  SSSUM(I)=SSUM2
  TSSUM(I)=TSSUM(I-1)+DPT*(SSSUM(I)+SSSUM(I-1))/2.
34 CONTINUE
C
C
  AAASUM=1.0
  DO 110 I=1,20
  SUM2=SQRT(4.*SI*PT)/2.
  ASSLM=SUM2**2.*I
  AAASUM=(ASSUM/(AK(I)**2.))+AAASUM
110 CONTINUE
  PPT=TAU+TAUP
  XXX=AAASUM*EXP(-SI-PPT)
  DO 250 I=1,501
  XXOUT(I)=XCUT(501)-XXX-TSSUM(I)
250 CONTINUE
C
C
C
  WRITE(6,60)
60 FORMAT('1',8X,'TIME',12X,'TPRIME',9X,'TAU',7X,
*'EFFLUENT CONC.')
  DO 121 I=1,501,20
  WRITE(6,132)REALT(I),TPRIME(I),TTAU(I),XOUT(I)
121 CONTINUE
  DO 122 I=1,501,20

```

```
WRITE(6,132)RREALT(I),TTPRIM(I),TTAUP(I),XXOUT(I)
132 FORMAT(5X,F11.5,5X,F11.5,5X,F9.5,5X,F9.5)
122 CONTINUE
506 CONTINUE
STOP
END
```

APPENDIX VI

COMPUTER DEVELOPED BREAKTHROUGH DATA

TABLE 28

EFFECT OF MASS TRANSFER COEFFICIENT
OF EFFLUENT CONCENTRATION

$$a = 1000, m = 1.0$$

TABLE 28
 $\epsilon \lambda = 0.01$

TIME	T _{PRIME}	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
39.76511	9.91999	0.16000	0.12623
49.68510	19.83998	0.32000	0.20074
59.60510	29.75998	0.48000	0.27403
69.52510	39.67998	0.64000	0.34481
79.44510	49.59998	0.80000	0.41224
89.36510	59.51997	0.96000	0.47575
99.28505	69.43993	1.12000	0.53502
109.20505	79.35992	1.28000	0.58994
119.12503	89.27991	1.44000	0.64047
129.04507	99.19995	1.60000	0.68673
138.96507	109.11995	1.76000	0.72887
148.88506	119.03993	1.92000	0.76710
158.80505	128.95993	2.08000	0.80165
168.72504	138.87991	2.24000	0.83277
178.64503	148.79991	2.40000	0.86073
188.56502	158.71989	2.56000	0.88578
198.48502	168.63989	2.72000	0.91816
208.40500	178.55988	2.88000	0.92812
218.32506	188.47993	3.04000	0.94589
228.24504	198.39992	3.20000	0.96168
238.16504	208.31992	3.36000	0.97568
248.08502	218.23990	3.52000	0.98807
258.00488	228.15990	3.68000	0.99904
267.92480	238.07988	3.84000	1.00872
277.84497	247.99988	4.00000	1.01726
277.84497	247.99988	4.00000	1.01719
282.80493	252.95987	4.08000	0.97932
287.76464	257.91967	4.16000	0.94213
292.72460	262.87963	4.24000	0.91482
297.68481	267.83984	4.32000	0.86761
302.64477	272.79980	4.40000	0.83073
307.60473	277.75976	4.48000	0.79433
312.56469	282.71972	4.56000	0.75857
317.52465	287.67968	4.64000	0.72355
322.48461	292.63964	4.72000	0.68937
327.44458	297.59960	4.80000	0.65612
332.40478	302.55981	4.88000	0.62385
337.36474	307.51977	4.96000	0.59261
342.32470	312.47973	5.04000	0.56243
347.28466	317.43969	5.12000	0.53333
352.24462	322.39965	5.20000	0.50533
357.20458	327.35961	5.28000	0.47842
362.16455	332.31958	5.36000	0.45261
367.12475	337.27978	5.44000	0.42789
372.08471	342.23974	5.52000	0.40423
377.04467	347.19970	5.60000	0.38163
382.00463	352.15966	5.68000	0.36006
386.96459	357.11962	5.76000	0.33949
391.92456	362.07958	5.84000	0.31990
396.88452	367.03955	5.92000	0.30126
401.84472	371.99975	6.00000	0.28354

TABLE 28 CONTINUED

$$\epsilon \lambda = 0.02$$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.04186
34.80511	4.95999	0.16000	0.08174
39.76511	9.91999	0.32000	0.12350
44.72510	14.87999	0.48000	0.16801
49.68510	19.83998	0.64000	0.21354
54.64510	24.79997	0.80000	0.25881
59.60509	29.75996	0.96000	0.30291
64.56506	34.71994	1.12000	0.34520
69.52505	39.67993	1.28000	0.38524
74.48505	44.63992	1.44000	0.42278
79.44507	49.59995	1.60000	0.45768
84.40506	54.55994	1.76000	0.48990
89.36507	59.51994	1.92000	0.51947
94.32506	64.47993	2.08000	0.54647
99.28505	69.43993	2.24000	0.57101
104.24504	74.39992	2.40000	0.59324
109.20503	79.35991	2.56000	0.61329
114.16502	84.31990	2.72000	0.63132
119.12502	89.27989	2.88000	0.64750
124.08504	94.23991	3.04000	0.66198
129.04503	99.19991	3.20000	0.67490
134.00502	104.15990	3.36000	0.68641
138.96501	109.11989	3.52000	0.69665
143.92500	114.07988	3.68000	0.70574
148.88501	119.03989	3.84000	0.71379
153.84500	123.99988	4.00000	0.72092
153.84500	123.99988	4.00000	0.72086
156.32500	126.47987	4.08000	0.70172
158.80499	128.95987	4.16000	0.68256
161.28499	131.43987	4.24000	0.66216
163.76498	133.91986	4.32000	0.64081
166.24498	136.39986	4.40000	0.61878
168.72498	138.87985	4.48000	0.59630
171.20497	141.35985	4.56000	0.57358
173.68497	143.83984	4.64000	0.55077
176.16496	146.31984	4.72000	0.52804
178.64496	148.79984	4.80000	0.50550
181.12495	151.27983	4.88000	0.48325
183.60495	153.75983	4.96000	0.46140
186.08495	156.23982	5.04000	0.43999
188.56494	158.71982	5.12000	0.41911
191.04494	161.19981	5.20000	0.39879
193.52493	163.67981	5.28000	0.37907
196.00493	166.15981	5.36000	0.35997
198.48492	168.63980	5.44000	0.34153
200.96492	171.11980	5.52000	0.32374
203.44492	173.59979	5.60000	0.30663
205.92491	176.07979	5.68000	0.29019
208.40491	178.55978	5.76000	0.27441
210.88492	181.03979	5.84000	0.25930
213.36491	183.51979	5.92000	0.24484
215.84491	185.99979	6.00000	0.23103

TABLE 28 CONTINUED
 $\epsilon \lambda = 0.03$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.02776
33.15178	3.30666	0.16000	0.04948
36.45845	6.61333	0.32000	0.07207
39.76511	9.91999	0.48000	0.09742
43.07178	13.22666	0.64000	0.12422
46.37843	16.53331	0.80000	0.15149
49.68510	19.83998	0.96000	0.17851
52.99174	23.14662	1.12000	0.20474
56.29842	26.45329	1.28000	0.22984
59.60507	29.75995	1.44000	0.25357
62.91176	33.06664	1.60000	0.27577
66.21841	36.37329	1.76000	0.29640
69.52509	39.67996	1.92000	0.31541
72.83174	42.98662	2.08000	0.33285
76.13840	46.29327	2.24000	0.34876
79.44507	49.59995	2.40000	0.36321
82.75172	52.90660	2.56000	0.37629
86.05838	56.21326	2.72000	0.38808
89.36505	59.51993	2.88000	0.39868
92.67174	62.82661	3.04000	0.40819
95.97839	66.13327	3.20000	0.41669
99.28505	69.43993	3.36000	0.42428
102.59172	72.74660	3.52000	0.43104
105.89838	76.05325	3.68000	0.43705
109.20505	79.35992	3.84000	0.44238
112.51170	82.66658	4.00000	0.44710
112.51170	82.66658	4.00000	0.44707
114.16502	84.31990	4.08000	0.43689
115.81836	85.97324	4.16000	0.42715
117.47169	87.62657	4.24000	0.41630
119.12502	89.27989	4.32000	0.40456
120.77835	90.93323	4.40000	0.39214
122.43169	92.58656	4.48000	0.37921
124.08501	94.23988	4.56000	0.36593
125.73834	95.89322	4.64000	0.35241
127.39168	97.54655	4.72000	0.33879
129.04501	99.19989	4.80000	0.32514
130.69833	100.85321	4.88000	0.31157
132.35167	102.50655	4.96000	0.29813
134.00500	104.15988	5.04000	0.28489
135.65833	105.81320	5.12000	0.27190
137.31166	107.46654	5.20000	0.25919
138.96500	109.11987	5.28000	0.24680
140.61832	110.77319	5.36000	0.23475
142.27165	112.42653	5.44000	0.22307
143.92499	114.07986	5.52000	0.21177
145.57831	115.73318	5.60000	0.20087
147.23164	117.38652	5.68000	0.19035
148.88498	119.03986	5.76000	0.18025
150.53831	120.69319	5.84000	0.17054
152.19164	122.34651	5.92000	0.16123
153.84497	123.99985	6.00000	0.15231

TABLE 28 CONTINUED
 $\epsilon \lambda = 0.04$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.01661
32.32512	2.48000	0.16000	0.02931
34.80511	4.96000	0.32000	0.04123
37.28511	7.44000	0.48000	0.05510
39.76512	9.92000	0.64000	0.07007
42.24512	12.40000	0.80000	0.08553
44.72511	14.88000	0.96000	0.10099
47.20511	17.35999	1.12000	0.11612
49.68510	19.83998	1.28000	0.13069
52.16510	22.31998	1.44000	0.14452
54.64511	24.79999	1.60000	0.15751
57.12511	27.27998	1.76000	0.16962
59.60510	29.75998	1.92000	0.18081
62.08510	32.23997	2.08000	0.19110
64.56509	34.71997	2.24000	0.20051
67.04510	37.19998	2.40000	0.20907
69.52510	39.67998	2.56000	0.21682
72.00510	42.15997	2.72000	0.22383
74.48509	44.63997	2.88000	0.23013
76.96510	47.11998	3.04000	0.23579
79.44510	49.59998	3.20000	0.24086
81.92509	52.07997	3.36000	0.24538
84.40511	54.55998	3.52000	0.24942
86.88510	57.03998	3.68000	0.25301
89.36510	59.51997	3.84000	0.25619
91.84509	61.99997	4.00000	0.25902
91.84509	61.99997	4.00000	0.25900
93.08508	63.23996	4.08000	0.25311
94.32509	64.47997	4.16000	0.24821
95.56508	65.71996	4.24000	0.24256
96.80508	66.95996	4.32000	0.23629
98.04507	68.19995	4.40000	0.22955
99.28508	69.43996	4.48000	0.22243
100.52509	70.67996	4.56000	0.21503
101.76508	71.91995	4.64000	0.20745
103.00508	73.15996	4.72000	0.19975
104.24507	74.39995	4.80000	0.19200
105.48508	75.63995	4.88000	0.18424
106.72508	76.87996	4.96000	0.17653
107.96507	78.11995	5.04000	0.16891
109.20508	79.35995	5.12000	0.16140
110.44507	80.59995	5.20000	0.15404
111.68507	81.83995	5.28000	0.14684
112.92506	83.07994	5.36000	0.13982
114.16507	84.31995	5.44000	0.13301
115.40506	85.55994	5.52000	0.12640
116.64507	86.79994	5.60000	0.12001
117.88507	88.03995	5.68000	0.11385
119.12506	89.27994	5.76000	0.10791
120.36507	90.51994	5.84000	0.10220
121.60506	91.75993	5.92000	0.09671
122.84506	92.99994	6.00000	0.09146

TABLE 28 CONTINUED

 $\epsilon \lambda = 0.05$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.00938
31.82912	1.98400	0.16000	0.01763
33.81311	3.96800	0.32000	0.02380
35.79712	5.95200	0.48000	0.03117
37.78111	7.93600	0.64000	0.03926
39.76511	9.92000	0.80000	0.04768
41.74911	11.90400	0.96000	0.05617
43.73311	13.88799	1.12000	0.06451
45.71710	15.87198	1.28000	0.07258
47.70110	17.85597	1.44000	0.08026
49.68510	19.83998	1.60000	0.08749
51.66911	21.82399	1.76000	0.09424
53.65311	23.80798	1.92000	0.10050
55.63710	25.79198	2.08000	0.10625
57.62109	27.77597	2.24000	0.11152
59.60510	29.75998	2.40000	0.11632
61.58910	31.74397	2.56000	0.12067
63.57309	33.72797	2.72000	0.12461
65.55710	35.71198	2.88000	0.12816
67.54111	37.69598	3.04000	0.13134
69.52510	39.67998	3.20000	0.13419
71.50909	41.66397	3.36000	0.13674
73.49310	43.64798	3.52000	0.13902
75.47710	45.63197	3.68000	0.14104
77.46109	47.61597	3.84000	0.14284
79.44508	49.59996	4.00000	0.14443
79.44508	49.59996	4.00000	0.14442
80.43707	50.59195	4.08000	0.14057
81.42908	51.58395	4.16000	0.13813
82.42107	52.57594	4.24000	0.13523
83.41307	53.56795	4.32000	0.13196
84.40508	54.55995	4.40000	0.12839
85.39706	55.55194	4.48000	0.12459
86.38907	56.54395	4.56000	0.12061
87.38107	57.53595	4.64000	0.11650
88.37306	58.52794	4.72000	0.11231
89.36507	59.51994	4.80000	0.10808
90.35707	60.51195	4.88000	0.10383
91.34906	61.50394	4.96000	0.09959
92.34106	62.49594	5.04000	0.09539
93.33307	63.48795	5.12000	0.09124
94.32506	64.47993	5.20000	0.08717
95.31706	65.47194	5.28000	0.08318
96.30907	66.46394	5.36000	0.07929
97.30106	67.45593	5.44000	0.07553
98.29306	68.44794	5.52000	0.07183
99.28505	69.43993	5.60000	0.06827
100.27705	70.43193	5.68000	0.06483
101.26906	71.42393	5.76000	0.06152
102.26105	72.41592	5.84000	0.05833
103.25305	73.40793	5.92000	0.05526
104.24506	74.39993	6.00000	0.05232

TABLE 28 CONTINUED

 $\epsilon \lambda = 0.06$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.00510
31.49844	1.65333	0.16000	0.01117
33.15178	3.30666	0.32000	0.01431
34.80511	4.96000	0.48000	0.01816
36.45845	6.61333	0.64000	0.02241
38.11179	8.26666	0.80000	0.02688
39.76511	9.92000	0.96000	0.03141
41.41844	11.57332	1.12000	0.03587
43.07176	13.22665	1.28000	0.04020
44.72510	14.87998	1.44000	0.04432
46.37845	16.53333	1.60000	0.04822
48.03177	18.18665	1.76000	0.05186
49.68510	19.83998	1.92000	0.05524
51.33844	21.49332	2.08000	0.05835
52.99176	23.14664	2.24000	0.06120
54.64510	24.79997	2.40000	0.06380
56.29843	26.45331	2.56000	0.06615
57.95177	28.10664	2.72000	0.06829
59.60509	29.75996	2.88000	0.07021
61.25844	31.41331	3.04000	0.07194
62.91177	33.06665	3.20000	0.07348
64.56509	34.71997	3.36000	0.07487
66.21843	36.37331	3.52000	0.07610
67.87177	38.02664	3.68000	0.07720
69.52509	39.67996	3.84000	0.07818
71.17842	41.33330	4.00000	0.07904
71.17842	41.33330	4.00000	0.07904
72.00508	42.15996	4.08000	0.07616
72.83174	42.98662	4.16000	0.07495
73.65842	43.81329	4.24000	0.07348
74.48508	44.63995	4.32000	0.07180
75.31174	45.46661	4.40000	0.06995
76.13841	46.29329	4.48000	0.06796
76.96507	47.11995	4.56000	0.06587
77.79175	47.94662	4.64000	0.06370
78.61841	48.77328	4.72000	0.06148
79.44507	49.59995	4.80000	0.05923
80.27174	50.42662	4.88000	0.05697
81.09840	51.25328	4.96000	0.05471
81.92506	52.07994	5.04000	0.05246
82.75174	52.90662	5.12000	0.05024
83.57840	53.73328	5.20000	0.04806
84.40506	54.55994	5.28000	0.04592
85.23174	55.38661	5.36000	0.04383
86.05840	56.21327	5.44000	0.04179
86.88506	57.03993	5.52000	0.03981
87.71173	57.86661	5.60000	0.03790
88.53839	58.69327	5.68000	0.03604
89.36507	59.51994	5.76000	0.03426
90.19173	60.34660	5.84000	0.03254
91.01839	61.17326	5.92000	0.03088
91.84506	61.99994	6.00000	0.02929

TABLE 28 CONTINUED

$$\epsilon \lambda = 0.07$$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.00270
31.26225	1.41714	0.16000	0.00770
32.67940	2.83428	0.32000	0.00929
34.09654	4.25143	0.48000	0.01126
35.51369	5.66857	0.64000	0.01346
36.93083	7.08571	0.80000	0.01579
38.34798	8.50285	0.96000	0.01815
39.76511	9.91999	1.12000	0.02048
41.18225	11.33713	1.28000	0.02275
42.59940	12.75427	1.44000	0.02492
44.01654	14.17142	1.60000	0.02697
45.43369	15.58857	1.76000	0.02888
46.85083	17.00571	1.92000	0.03066
48.26796	18.42284	2.08000	0.03230
49.68510	19.83998	2.24000	0.03381
51.10225	21.25713	2.40000	0.03518
52.51939	22.67427	2.56000	0.03642
53.93654	24.09142	2.72000	0.03755
55.35367	25.50854	2.88000	0.03856
56.77083	26.92570	3.04000	0.03948
58.18796	28.34283	3.20000	0.04030
59.60510	29.75998	3.36000	0.04103
61.02225	31.17712	3.52000	0.04168
62.43939	32.59427	3.68000	0.04226
63.85654	34.01141	3.84000	0.04278
65.27367	35.42854	4.00000	0.04324
65.27367	35.42854	4.00000	0.04324
65.98222	36.84567	4.16000	0.04082
66.69080	36.84567	4.16000	0.04023
67.39937	37.55424	4.24000	0.03949
68.10794	38.26282	4.32000	0.03864
68.81651	38.97139	4.40000	0.03769
69.52509	39.67996	4.48000	0.03667
70.23366	40.38853	4.56000	0.03559
70.94223	41.09711	4.64000	0.03447
71.65080	41.80568	4.72000	0.03331
72.35938	42.51425	4.80000	0.03214
73.06793	43.22281	4.88000	0.03096
73.77650	43.93138	4.96000	0.02978
74.48508	44.63995	5.04000	0.02861
75.19365	45.34853	5.12000	0.02744
75.90222	46.05710	5.20000	0.02630
76.61079	46.76567	5.28000	0.02518
77.31937	47.47424	5.36000	0.02408
78.02794	48.18282	5.44000	0.02301
78.73651	48.89139	5.52000	0.02197
79.44507	49.59995	5.60000	0.02096
80.15364	50.30852	5.68000	0.01999
80.86221	51.01709	5.76000	0.01904
81.57079	51.72566	5.84000	0.01814
82.27936	52.43423	5.92000	0.01727
82.98793	53.14281	6.00000	0.01643

TABLE 29

EFFECT OF EQUILIBRIUM CONSTANT ON EFFLUENT CONCENTRATION

$$a = 1000 \quad K_x = 0.00001$$

TABLE 29 CONTINUED

m = 0.8

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
42.24512	12.39999	0.16000	0.12623
54.64511	24.79999	0.32000	0.20074
67.04510	37.19998	0.48000	0.27403
79.44511	49.59999	0.64000	0.34431
91.84511	61.99998	0.80000	0.41224
104.24510	74.39998	0.96000	0.47575
116.64505	86.79993	1.12000	0.53502
129.04504	99.19992	1.28000	0.58994
141.44504	111.59991	1.44000	0.64047
153.84509	123.99997	1.60000	0.68673
166.24509	136.39996	1.76000	0.72887
178.64508	148.79996	1.92000	0.76710
191.04507	161.19995	2.08000	0.80165
203.44505	173.59993	2.24000	0.83277
215.84505	185.99992	2.40000	0.86073
228.24504	198.39992	2.56000	0.88578
240.64503	210.79991	2.72000	0.90816
253.04501	223.19989	2.88000	0.92812
265.44506	235.59996	3.04000	0.94589
277.84497	247.99995	3.20000	0.96168
290.24487	260.39990	3.36000	0.97568
302.64477	272.79980	3.52000	0.98807
315.04467	285.19970	3.68000	0.99904
327.44482	297.59985	3.84000	1.00872
339.84472	309.99975	4.00000	1.01726
339.84472	309.99975	4.00000	1.01725
355.34448	325.49951	4.20000	0.92191
370.84448	340.99951	4.40000	0.82916
386.34448	356.49951	4.60000	0.73939
401.84448	371.99951	4.80000	0.65455
417.34448	387.49951	5.00000	0.57582
432.84448	402.99951	5.20000	0.50376
448.34448	418.49951	5.40000	0.43854
463.84448	433.99951	5.60000	0.38006
479.34448	449.49951	5.80000	0.32800
494.84448	464.99951	6.00000	0.28197
510.34448	480.49951	6.20000	0.24149
525.84448	495.99951	6.40000	0.20606
541.34448	511.49951	6.60000	0.17517
556.84448	526.99951	6.80000	0.14836
572.34448	542.49951	7.00000	0.12514
587.84448	557.99951	7.20000	0.10511
603.34448	573.49951	7.40000	0.08787
618.84448	588.99951	7.60000	0.07306
634.34448	604.49951	7.80000	0.06038
649.84448	619.99951	8.00000	0.04953
665.34448	635.49951	8.20000	0.04027
680.84448	650.99951	8.40000	0.03237
696.34448	666.49951	8.60000	0.02566
711.84448	681.99951	8.80000	0.01996
727.34448	697.49951	9.00000	0.01512

TABLE 29

m = 0.6

TIME	T _{PRIME}	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
46.37845	16.53333	0.16000	0.12623
62.91179	33.06667	0.32000	0.20074
79.44511	49.59999	0.48000	0.27403
95.97845	66.13333	0.64000	0.34481
112.51178	82.66666	0.80000	0.41224
129.04512	99.20000	0.96000	0.47575
145.57838	115.73326	1.12000	0.53502
162.11171	132.26659	1.28000	0.58994
178.64503	148.79991	1.44000	0.64047
195.17845	165.33333	1.60000	0.68673
211.71178	181.86665	1.76000	0.72837
228.24510	198.39998	1.92000	0.76710
244.77843	214.93330	2.08000	0.80165
261.31152	231.46663	2.24000	0.83277
277.84497	247.99995	2.40000	0.86073
294.37817	264.53320	2.56000	0.88578
310.91137	281.06640	2.72000	0.90816
327.44482	297.59985	2.88000	0.92812
343.97827	314.13330	3.04000	0.94589
360.51147	330.66650	3.20000	0.96168
377.04492	347.19995	3.36000	0.97568
393.57812	363.73315	3.52000	0.98807
410.11157	380.26660	3.68000	0.99904
426.64477	396.79980	3.84000	1.00872
443.17822	413.33325	4.00000	1.01726
463.17822	413.33325	4.00000	1.01725
463.84472	433.99975	4.20000	0.92191
484.51147	454.66650	4.40000	0.82916
505.17822	475.33325	4.60000	0.73939
525.84472	495.99975	4.80000	0.65455
546.51147	516.66650	5.00000	0.57582
567.17797	537.33300	5.20000	0.50376
587.84472	557.99975	5.40000	0.43854
608.51147	578.66650	5.60000	0.38006
629.17797	599.33300	5.80000	0.32800
649.84472	619.99975	6.00000	0.28197
670.51147	640.66650	6.20000	0.24149
691.17797	661.33300	6.40000	0.20606
711.84472	681.99975	6.60000	0.17517
732.51147	702.66650	6.80000	0.14836
753.17822	723.33325	7.00000	0.12514
773.84472	743.99975	7.20000	0.10511
794.51147	764.66650	7.40000	0.08787
815.17797	785.33300	7.60000	0.07306
835.84472	805.99975	7.80000	0.06038
856.51147	826.66650	8.00000	0.04953
877.17822	847.33325	8.20000	0.04027
897.84472	867.99975	8.40000	0.03237
918.51147	888.66650	8.60000	0.02566
939.17822	909.33325	8.80000	0.01996
959.84472	929.99975	9.00000	0.01512

TABLE 29 CONTINUED

m = 1.2

TIME	T _{PRIME}	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
38.11179	8.26666	0.16000	0.12623
46.37845	16.53333	0.32000	0.20074
54.64511	24.79999	0.48000	0.27403
62.91179	33.06667	0.64000	0.34491
71.17845	41.33333	0.80000	0.41224
79.44511	49.59999	0.96000	0.47575
87.71175	57.86662	1.12000	0.53502
95.97841	66.13329	1.28000	0.58994
104.24507	74.39995	1.44000	0.64047
112.51178	82.66666	1.60000	0.68673
120.77844	90.93332	1.76000	0.72887
129.04510	99.19998	1.92000	0.76710
137.31177	107.46664	2.08000	0.80165
145.57843	115.73331	2.24000	0.83277
153.84509	123.99997	2.40000	0.86073
162.11176	132.26663	2.56000	0.88578
170.37842	140.53329	2.72000	0.90816
178.64508	148.79996	2.88000	0.92812
186.91179	157.06667	3.04000	0.94589
195.17845	165.33333	3.20000	0.96168
203.44511	173.59999	3.36000	0.97568
211.71178	181.86665	3.52000	0.98807
219.97844	190.13332	3.68000	0.99904
228.24510	198.39998	3.84000	1.00872
236.51176	206.66664	4.00000	1.01726
236.51176	206.66664	4.00000	1.01725
246.84509	216.99997	4.20000	0.92191
257.17822	227.33330	4.40000	0.82916
267.51171	237.66664	4.60000	0.73939
277.84497	247.99997	4.80000	0.65455
288.17822	258.33325	5.00000	0.57582
298.51147	268.66650	5.20000	0.50376
308.84472	278.99975	5.40000	0.43854
319.17822	289.33325	5.60000	0.38006
329.51147	299.66650	5.80000	0.32800
339.84472	309.99975	6.00000	0.28197
350.17822	320.33325	6.20000	0.24149
360.51147	330.66650	6.40000	0.20606
370.84472	340.99975	6.60000	0.17517
381.17822	351.33325	6.80000	0.14836
391.51147	361.66650	7.00000	0.12514
401.84472	371.99975	7.20000	0.10511
412.17822	382.33325	7.40000	0.08787
422.51147	392.66650	7.60000	0.07306
432.84472	402.99975	7.80000	0.06038
443.17822	413.33325	8.00000	0.04953
453.51147	423.66650	8.20000	0.04027
463.84472	433.99975	8.40000	0.03237
474.17822	444.33325	8.60000	0.02566
484.51147	454.66650	8.80000	0.01996
494.84472	464.99975	9.00000	0.01512

TABLE 29 CONTINUED

$$m = 1.4$$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
36.93083	7.08571	0.16000	0.12623
44.01654	14.17142	0.32000	0.20074
51.10225	21.25713	0.48000	0.27403
58.18797	28.34285	0.64000	0.34481
65.27368	35.42856	0.80000	0.41224
72.35939	42.51427	0.96000	0.47575
79.44507	49.59995	1.12000	0.53502
86.53078	56.68565	1.28000	0.58994
93.61649	63.77136	1.44000	0.64047
100.70224	70.85712	1.60000	0.68673
107.78795	77.94283	1.76000	0.72887
114.87366	85.02853	1.92000	0.76710
121.95937	92.11424	2.08000	0.80165
129.04507	99.19995	2.24000	0.83277
136.13078	106.28566	2.40000	0.86073
143.21649	113.37137	2.56000	0.88578
150.30220	120.45708	2.72000	0.90816
157.38791	127.54279	2.88000	0.92812
164.47366	134.62854	3.04000	0.94589
171.55937	141.71425	3.20000	0.96168
178.64508	148.79996	3.36000	0.97568
185.73079	155.88567	3.52000	0.98807
192.81650	162.97137	3.68000	0.99904
199.90221	170.05708	3.84000	1.00872
206.98792	177.14279	4.00000	1.01726
206.98792	177.14279	4.00000	1.01725
215.84505	185.99992	4.20000	0.92191
224.70219	194.85707	4.40000	0.82916
233.55933	203.71420	4.60000	0.73939
242.41647	212.57135	4.80000	0.65455
251.27362	221.42850	5.00000	0.57582
260.13061	230.28560	5.20000	0.50376
268.98779	239.14278	5.40000	0.43854
277.84497	247.99991	5.60000	0.38006
286.70190	256.85693	5.80000	0.32800
295.55908	265.71411	6.00000	0.28197
304.41625	274.57128	6.20000	0.24149
313.27319	283.42822	6.40000	0.20606
322.13037	292.28540	6.60000	0.17517
330.98754	301.14257	6.80000	0.14836
339.84472	309.99975	7.00000	0.12514
348.70190	318.85693	7.20000	0.10511
357.55908	327.71411	7.40000	0.08787
366.41625	336.57128	7.60000	0.07306
375.27319	345.42822	7.80000	0.06038
384.13037	354.28540	8.00000	0.04953
392.98754	363.14257	8.20000	0.04027
401.84472	371.99975	8.40000	0.03237
410.70190	380.85693	8.60000	0.02566
419.55908	389.71411	8.80000	0.01996
428.41625	398.57128	9.00000	0.01512

TABLE 29 CONTINUED

m = 1.8

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
36.04512	6.21000	0.16000	0.12623
42.24512	12.40000	0.32000	0.20074
48.44511	18.59999	0.48000	0.27403
54.64511	24.79999	0.64000	0.34431
60.84512	31.00000	0.80000	0.41224
67.04512	37.20000	0.96000	0.47575
73.24509	43.39996	1.12000	0.53502
79.44508	49.59996	1.28000	0.58994
85.64508	55.79996	1.44000	0.64047
91.84512	62.00000	1.60000	0.68673
98.04512	68.20000	1.76000	0.72887
104.24512	74.39999	1.92000	0.76710
110.44511	80.59999	2.08000	0.80165
116.64511	86.79999	2.24000	0.83277
122.84511	92.99998	2.40000	0.86073
129.04509	99.19997	2.56000	0.88578
135.24509	105.39996	2.72000	0.90816
141.44508	111.59996	2.88000	0.92812
147.64513	117.80000	3.04000	0.94589
153.84512	124.00000	3.20000	0.96168
160.04512	130.20000	3.36000	0.97568
166.24512	136.39999	3.52000	0.98807
172.44511	142.59999	3.68000	0.99904
178.64511	148.79999	3.84000	1.00872
184.84511	154.99998	4.00000	1.01726
184.84511	154.99998	4.00000	1.01725
192.59511	162.74998	4.20000	0.92191
200.34511	170.49998	4.40000	0.82916
208.09511	178.24998	4.60000	0.73939
215.84511	185.99998	4.80000	0.65455
223.59511	193.74998	5.00000	0.57582
231.34508	201.49995	5.20000	0.50376
239.09511	209.24998	5.40000	0.43854
246.84511	216.99998	5.60000	0.38006
254.59509	224.74997	5.80000	0.32800
262.34497	232.49997	6.00000	0.28197
270.09497	240.24997	6.20000	0.24149
277.84497	247.99997	6.40000	0.20606
285.59497	255.75000	6.60000	0.17517
293.34472	263.49975	6.80000	0.14836
301.09472	271.24975	7.00000	0.12514
308.84472	278.99975	7.20000	0.10511
316.59472	286.74975	7.40000	0.08787
324.34472	294.49975	7.60000	0.07306
332.09472	302.24975	7.80000	0.06038
339.84497	310.00000	8.00000	0.04953
347.59497	317.75000	8.20000	0.04027
355.34497	325.50000	8.40000	0.03237
363.09472	333.24975	8.60000	0.02566
370.84472	340.99975	8.80000	0.01996
378.59472	348.74975	9.00000	0.01512

TABLE 29 CONTINUED

m = 2.0

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
34.80511	4.96000	0.16000	0.12623
39.76511	9.92000	0.32000	0.20074
44.72511	14.87999	0.48000	0.27403
49.68510	19.83998	0.64000	0.34461
54.64511	24.79999	0.80000	0.41224
59.60510	29.75998	0.96000	0.47575
64.56508	34.71996	1.12000	0.53502
69.52509	39.67996	1.28000	0.58994
74.48508	44.63995	1.44000	0.64047
79.44510	49.59998	1.60000	0.68673
84.40509	54.55997	1.76000	0.72887
89.36508	59.51996	1.92000	0.76710
94.32509	64.47997	2.08000	0.80165
99.28508	69.43996	2.24000	0.83277
104.24507	74.39995	2.40000	0.86073
109.20506	79.35994	2.56000	0.88578
114.16507	84.31995	2.72000	0.90816
119.12506	89.27994	2.88000	0.92812
124.08508	94.23996	3.04000	0.94589
129.04507	99.19995	3.20000	0.96168
134.00508	104.15996	3.36000	0.97568
138.96507	109.11995	3.52000	0.98807
143.92506	114.07994	3.68000	0.99904
148.88506	119.03993	3.84000	1.00872
153.84506	123.99994	4.00000	1.01726
153.84506	123.99994	4.00000	1.01725
160.04506	130.19994	4.20000	0.92191
166.24506	136.39993	4.40000	0.82916
172.44505	142.59993	4.60000	0.73939
178.64505	148.79993	4.80000	0.65455
184.84505	154.99992	5.00000	0.57582
191.04501	161.19989	5.20000	0.50376
197.24504	167.39992	5.40000	0.43854
203.44504	173.59991	5.60000	0.38006
209.64503	179.79991	5.80000	0.32800
215.84503	185.99991	6.00000	0.28197
222.04501	192.19989	6.20000	0.24149
228.24501	198.39989	6.40000	0.20606
234.44504	204.59991	6.60000	0.17517
240.64503	210.79991	6.80000	0.14836
246.84503	216.99991	7.00000	0.12514
253.04501	223.19989	7.20000	0.10511
259.24487	229.39989	7.40000	0.08787
265.44482	235.59988	7.60000	0.07306
271.64477	241.79988	7.80000	0.06038
277.84497	247.99991	8.00000	0.04953
284.04492	254.19989	8.20000	0.04027
290.24462	260.39965	8.40000	0.03237
296.44482	266.59985	8.60000	0.02566
302.64477	272.79980	8.80000	0.01996
308.84472	278.99975	9.00000	0.01512

TABLE 29 CONTINUED

m = 2.2

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
34.35420	4.50909	0.16000	0.12623
38.86331	9.01818	0.32000	0.20074
43.37239	13.52727	0.48000	0.27403
47.88143	18.03636	0.64000	0.34491
52.39056	22.54544	0.80000	0.41224
56.89966	27.05453	0.96000	0.47575
61.40872	31.56360	1.12000	0.53502
65.91782	36.07269	1.28000	0.58994
70.42691	40.58179	1.44000	0.64047
74.93602	45.09090	1.60000	0.68673
79.44510	49.59998	1.76000	0.72887
83.95419	54.10907	1.92000	0.76710
88.46329	58.61816	2.08000	0.80165
92.97237	63.12724	2.24000	0.83277
97.48146	67.63634	2.40000	0.86073
101.99054	72.14542	2.56000	0.88578
106.49963	76.65451	2.72000	0.90816
111.00871	81.16359	2.88000	0.92812
115.51784	85.67271	3.04000	0.94589
120.02692	90.18179	3.20000	0.96168
124.53601	94.69089	3.36000	0.97568
129.04509	99.19997	3.52000	0.98807
133.55418	103.70906	3.68000	0.99904
138.06326	108.21814	3.84000	1.00872
142.57236	112.72723	4.00000	1.01726
142.57236	112.72723	4.00000	1.01725
148.20871	118.36359	4.20000	0.92191
153.84508	123.99995	4.40000	0.82916
159.48145	129.63632	4.60000	0.73939
165.11780	135.27267	4.80000	0.65455
170.75417	140.90904	5.00000	0.57582
176.39050	146.54538	5.20000	0.50376
182.02689	152.18176	5.40000	0.43854
187.66325	157.81813	5.60000	0.38006
193.29961	163.45448	5.80000	0.32800
198.93597	169.09085	6.00000	0.28197
204.57233	174.72720	6.20000	0.24149
210.20869	180.36357	6.40000	0.20606
215.84508	185.99995	6.60000	0.17517
221.48143	191.63631	6.80000	0.14836
227.11780	197.27267	7.00000	0.12514
232.75415	202.90903	7.20000	0.10511
238.39052	208.54539	7.40000	0.08787
244.02687	214.18175	7.60000	0.07306
249.66324	219.81812	7.80000	0.06038
255.29962	225.45450	8.00000	0.04953
260.93599	231.09085	8.20000	0.04027
266.57226	236.72722	8.40000	0.03237
272.20849	242.36357	8.60000	0.02566
277.84497	247.99994	8.80000	0.01996
283.48120	253.63629	9.00000	0.01512

TABLE 29 CONTINUED
m = 2.4

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
33.97844	4.13333	0.16000	0.12623
38.11177	8.26666	0.32000	0.20074
42.24510	12.39999	0.48000	0.27403
46.37843	16.53331	0.64000	0.34481
50.51176	20.66664	0.80000	0.41224
54.64510	24.79997	0.96000	0.47575
58.77841	28.93329	1.12000	0.53502
62.91174	33.06662	1.28000	0.58904
67.04507	37.19995	1.44000	0.64047
71.17842	41.33330	1.60000	0.68673
75.31175	45.46663	1.76000	0.72887
79.44508	49.59996	1.92000	0.76710
83.57841	53.73329	2.08000	0.80165
87.71175	57.86662	2.24000	0.83277
91.84506	61.99994	2.40000	0.86073
95.97839	66.13327	2.56000	0.88578
100.11172	70.26660	2.72000	0.90816
104.24506	74.39993	2.88000	0.92812
108.37840	78.53328	3.04000	0.94589
112.51173	82.66661	3.20000	0.96168
116.64507	86.79994	3.36000	0.97568
120.77840	90.93327	3.52000	0.98807
124.91173	95.06660	3.68000	0.99904
129.04504	99.19992	3.84000	1.00872
133.17838	103.33325	4.00000	1.01726
133.17838	103.33325	4.00000	1.01725
138.34503	108.49991	4.20000	0.92191
143.51170	113.66658	4.40000	0.82916
148.67836	118.83324	4.60000	0.73939
153.84503	123.99991	4.80000	0.65455
159.01169	129.16656	5.00000	0.57582
164.17833	134.33321	5.20000	0.50376
169.34502	139.49989	5.40000	0.43854
174.51167	144.66655	5.60000	0.38006
179.67834	149.83322	5.80000	0.32800
184.84500	154.99988	6.00000	0.28197
190.01166	160.16653	6.20000	0.24149
195.17831	165.33319	6.40000	0.20606
200.34500	170.49988	6.60000	0.17517
205.51167	175.66655	6.80000	0.14836
210.67833	180.83321	7.00000	0.12514
215.84499	185.99986	7.20000	0.10511
221.01164	191.16652	7.40000	0.08787
226.17831	196.33319	7.60000	0.07306
231.34497	201.49985	7.80000	0.06038
236.51166	206.66653	8.00000	0.04953
241.67831	211.83319	8.20000	0.04027
246.84497	216.99985	8.40000	0.03237
252.01164	222.16652	8.60000	0.02566
257.17822	227.33318	8.80000	0.01996
262.34472	232.49983	9.00000	0.01512

TABLE 29 CONTINUED

m = 2.6

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
33.66049	3.81538	0.16000	0.12623
37.47588	7.63076	0.32000	0.20074
41.29126	11.44615	0.48000	0.27403
45.10664	15.26153	0.64000	0.34481
48.92203	19.07691	0.80000	0.41224
52.73741	22.89229	0.96000	0.47575
56.55278	26.70766	1.12000	0.53502
60.36815	30.52303	1.28000	0.58994
64.18353	34.33841	1.44000	0.64047
67.99893	38.15381	1.60000	0.68673
71.81432	41.96919	1.76000	0.72887
75.62970	45.78458	1.92000	0.76710
79.44507	49.59995	2.08000	0.80165
83.26045	53.41533	2.24000	0.83277
87.07584	57.23071	2.40000	0.86073
90.89122	61.04610	2.56000	0.88578
94.70659	64.86147	2.72000	0.90816
98.52197	68.67685	2.88000	0.92812
102.33737	72.49225	3.04000	0.94589
106.15276	76.30763	3.20000	0.96168
109.96814	80.12302	3.36000	0.97568
113.78351	83.93839	3.52000	0.98807
117.59889	87.75377	3.68000	0.99904
121.41428	91.56915	3.84000	1.00872
125.22966	95.38454	4.00000	1.01726
125.22966	95.38454	4.00000	1.01725
129.99889	100.15376	4.20000	0.92191
134.76811	104.92299	4.40000	0.82916
139.53734	109.69221	4.60000	0.73939
144.30656	114.46144	4.80000	0.65455
149.07579	119.23067	5.00000	0.57582
153.84500	123.99988	5.20000	0.50376
158.61424	128.76912	5.40000	0.43854
163.38347	133.53835	5.60000	0.38006
168.15269	138.30757	5.80000	0.32800
172.92192	143.07680	6.00000	0.28197
177.69115	147.84602	6.20000	0.24149
182.46037	152.61525	6.40000	0.20606
187.22961	157.38449	6.60000	0.17517
191.99884	162.15372	6.80000	0.14836
196.76807	166.92294	7.00000	0.12514
201.53729	171.69217	7.20000	0.10511
206.30652	176.46140	7.40000	0.08787
211.07574	181.23062	7.60000	0.07306
215.84497	185.99985	7.80000	0.06038
220.61421	190.76909	8.00000	0.04953
225.38344	195.53831	8.20000	0.04027
230.15266	200.30754	8.40000	0.03237
234.92189	205.07677	8.60000	0.02566
239.69112	209.84599	8.80000	0.01996
244.46034	214.61522	9.00000	0.01512

TABLE 29 CONTINUED
m = 2.8

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
33.38797	3.54285	0.16000	0.12623
36.93083	7.08571	0.32000	0.20074
40.47368	10.62857	0.48000	0.27403
44.01654	14.17142	0.64000	0.34491
47.55939	17.71428	0.80000	0.41224
51.10225	21.25713	0.96000	0.47575
54.64508	24.79996	1.12000	0.53502
58.18794	28.34282	1.28000	0.58994
61.73079	31.88567	1.44000	0.64047
65.27367	35.42854	1.60000	0.68673
68.81651	38.97139	1.76000	0.72887
72.35938	42.51425	1.92000	0.76710
75.90222	46.05710	2.08000	0.80165
79.44508	49.59996	2.24000	0.83277
82.98793	53.14281	2.40000	0.86073
86.53079	56.68567	2.56000	0.88578
90.07364	60.22852	2.72000	0.90816
93.61649	63.77136	2.88000	0.92812
97.15936	67.31424	3.04000	0.94589
100.70222	70.85710	3.20000	0.96168
104.24507	74.39995	3.36000	0.97568
107.78792	77.94279	3.52000	0.98807
111.33078	81.48566	3.68000	0.99904
114.87363	85.02850	3.84000	1.00872
118.41649	88.57137	4.00000	1.01726
118.41649	88.57137	4.00000	1.01725
122.84505	92.99992	4.20000	0.92191
127.27362	97.42850	4.40000	0.82916
131.70219	101.85707	4.60000	0.73939
136.13075	106.28563	4.80000	0.65455
140.55933	110.71420	5.00000	0.57582
144.98788	115.14276	5.20000	0.50376
149.41647	119.57135	5.40000	0.43854
153.84503	123.99991	5.60000	0.38006
158.27361	128.42848	5.80000	0.32800
162.70216	132.85704	6.00000	0.28197
167.13074	137.28561	6.20000	0.24149
171.55930	141.71417	6.40000	0.20606
175.98788	146.14276	6.60000	0.17517
180.41646	150.57133	6.80000	0.14836
184.84502	154.99989	7.00000	0.12514
189.27359	159.42847	7.20000	0.10511
193.70215	163.85703	7.40000	0.08787
198.13072	168.28560	7.60000	0.07306
202.55928	172.71416	7.80000	0.06038
206.98787	177.14275	8.00000	0.04953
211.41644	181.57132	8.20000	0.04027
215.84500	185.99988	8.40000	0.03237
220.27357	190.42845	8.60000	0.02566
224.70213	194.85701	8.80000	0.01996
229.13071	199.28558	9.00000	0.01512

TABLE 29 CONTINUED

m = 3.0

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
33.15178	3.30666	0.16000	0.12623
36.45345	6.61333	0.32000	0.20074
39.76511	9.91999	0.48000	0.27403
43.07178	13.22666	0.64000	0.34481
46.37843	16.53331	0.80000	0.41224
49.68510	19.83998	0.96000	0.47575
52.99174	23.14662	1.12000	0.53502
56.29842	26.45329	1.28000	0.58994
59.60507	29.75995	1.44000	0.64047
62.91176	33.06664	1.60000	0.68673
66.21841	36.37329	1.76000	0.72887
69.52509	39.67996	1.92000	0.76710
72.83174	42.98662	2.08000	0.80165
76.13840	46.29327	2.24000	0.83277
79.44507	49.59995	2.40000	0.86073
82.75172	52.90660	2.56000	0.88578
86.05838	56.21326	2.72000	0.90816
89.36505	59.51993	2.88000	0.92812
92.67174	62.82661	3.04000	0.94589
95.97839	66.13327	3.20000	0.96168
99.28505	69.43993	3.36000	0.97568
102.59172	72.74660	3.52000	0.98807
105.89838	76.05325	3.68000	0.99904
109.20505	79.35992	3.84000	1.00872
112.51170	82.66658	4.00000	1.01726
112.51170	82.66658	4.00000	1.01725
116.64502	86.79990	4.20000	0.92191
120.77835	90.93323	4.40000	0.82916
124.91168	95.06656	4.60000	0.73939
129.04501	99.19989	4.80000	0.65455
133.17834	103.33322	5.00000	0.57582
137.31166	107.46654	5.20000	0.50376
141.44501	111.59988	5.40000	0.43854
145.57834	115.73322	5.60000	0.38006
149.71165	119.86653	5.80000	0.32800
153.84499	123.99986	6.00000	0.28197
157.97832	128.13319	6.20000	0.24149
162.11165	132.26653	6.40000	0.20606
166.24500	136.39987	6.60000	0.17517
170.37831	140.53319	6.80000	0.14836
174.51164	144.66652	7.00000	0.12514
178.64497	148.79985	7.20000	0.10511
182.77831	152.93318	7.40000	0.08787
186.91162	157.06650	7.60000	0.07306
191.04495	161.19983	7.80000	0.06038
195.17830	165.33318	8.00000	0.04953
199.31163	169.46651	8.20000	0.04027
203.44496	173.59984	8.40000	0.03237
207.57828	177.73315	8.60000	0.02566
211.71161	181.86649	8.80000	0.01996
215.84494	185.99982	9.00000	0.01512

TABLE 29 CONTINUED
m = 3.2

TIME	T _{PRIME}	T _{AU}	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
32.94511	3.10000	0.16000	0.12623
36.04512	6.20000	0.32000	0.20074
39.14511	9.30000	0.48000	0.27403
42.24512	12.40000	0.64000	0.34491
45.34511	15.49999	0.80000	0.41224
48.44511	18.59999	0.96000	0.47575
51.54509	21.69997	1.12000	0.53502
54.64510	24.79997	1.28000	0.58994
57.74509	27.89996	1.44000	0.64047
60.84511	30.99996	1.60000	0.68673
63.94510	34.09998	1.76000	0.72887
67.04510	37.19998	1.92000	0.76710
70.14510	40.29997	2.08000	0.80165
73.24509	43.39996	2.24000	0.83277
76.34509	46.49997	2.40000	0.86073
79.44508	49.59996	2.56000	0.88578
82.54509	52.69997	2.72000	0.90816
85.64508	55.79996	2.88000	0.92812
88.74510	58.89998	3.04000	0.94589
91.84509	61.99997	3.20000	0.96168
94.94508	65.09996	3.36000	0.97568
98.04509	68.19997	3.52000	0.98807
101.14508	71.29996	3.68000	0.99904
104.24509	74.39996	3.84000	1.00872
107.34508	77.49995	4.00000	1.01726
107.34508	77.49995	4.00000	1.01725
111.22006	81.37494	4.20000	0.92191
115.09506	85.24994	4.40000	0.82916
118.97006	89.12494	4.60000	0.73939
122.84506	92.99994	4.80000	0.65455
126.72006	96.87494	5.00000	0.57582
130.59505	100.74992	5.20000	0.50376
134.47006	104.62494	5.40000	0.43854
138.34506	108.49994	5.60000	0.38006
142.22006	112.37494	5.80000	0.32800
146.09505	116.24992	6.00000	0.28197
149.97005	120.12492	6.20000	0.24149
153.84505	123.99992	6.40000	0.20606
157.72006	127.87494	6.60000	0.17517
161.59506	131.74994	6.80000	0.14836
165.47005	135.62492	7.00000	0.12514
169.34505	139.49992	7.20000	0.10511
173.22005	143.37492	7.40000	0.08787
177.09505	147.24992	7.60000	0.07306
180.97003	151.12491	7.80000	0.06038
184.84505	154.99992	8.00000	0.04953
188.72005	158.87492	8.20000	0.04027
192.59505	162.74992	8.40000	0.03237
196.47005	166.62492	8.60000	0.02566
200.34503	170.49991	8.80000	0.01996
204.22003	174.37491	9.00000	0.01512

TABLE 29 CONTINUED

$$m = 3.4$$

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
32.76276	2.91764	0.16000	0.12623
35.68040	5.83529	0.32000	0.20074
38.59805	8.75294	0.48000	0.27403
41.5157	11.67058	0.64000	0.34481
44.43335	14.58823	0.80000	0.41234
47.35098	17.50586	0.96000	0.47575
50.26862	20.42349	1.12000	0.53502
53.18626	23.34114	1.28000	0.58994
56.10391	26.25879	1.44000	0.64047
59.02155	29.17645	1.60000	0.68673
61.93921	32.09409	1.76000	0.72887
64.85686	35.01173	1.92000	0.76710
67.77451	37.92938	2.08000	0.80165
70.69214	40.84702	2.24000	0.83277
73.60979	43.76466	2.40000	0.86073
76.52744	46.68231	2.56000	0.88578
79.44507	49.59995	2.72000	0.90816
82.36272	52.51759	2.88000	0.92812
85.28038	55.43526	3.04000	0.94589
88.19803	58.35291	3.20000	0.96168
91.11566	61.27054	3.36000	0.97568
94.03331	64.18819	3.52000	0.98807
96.95096	67.10583	3.68000	0.99904
99.86861	70.02348	3.84000	1.00872
102.78624	72.94112	4.00000	1.01726
102.78624	72.94112	4.00000	1.01725
106.43329	76.58817	4.20000	0.92191
110.08035	80.23523	4.40000	0.82916
113.72740	83.88228	4.60000	0.73939
117.37447	87.52934	4.80000	0.65455
121.02151	91.17639	5.00000	0.57582
124.66856	94.82344	5.20000	0.50376
128.31563	98.47050	5.40000	0.43854
131.96269	102.11757	5.60000	0.38006
135.60974	105.76462	5.80000	0.32800
139.25679	109.41167	6.00000	0.28197
142.90385	113.05873	6.20000	0.24149
146.55090	116.70578	6.40000	0.20606
150.19798	120.35286	6.60000	0.17517
153.84503	123.99991	6.80000	0.14836
157.49208	127.64696	7.00000	0.12514
161.13914	131.29402	7.20000	0.10511
164.78619	134.94107	7.40000	0.08787
168.43324	138.58812	7.60000	0.07306
172.08031	142.23518	7.80000	0.06038
175.72737	145.88225	8.00000	0.04953
179.37444	149.52931	8.20000	0.04027
183.02148	153.17636	8.40000	0.03237
186.66853	156.82341	8.60000	0.02566
190.31560	160.47047	8.80000	0.01996
193.96265	164.11752	9.00000	0.01512

TABLE 29 CONTINUED

m = 3.6

TIME	T _{PRIME}	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
32.60066	2.75555	0.16000	0.12623
35.35622	5.51111	0.32000	0.20074
38.11177	8.26666	0.48000	0.27403
40.86732	11.02221	0.64000	0.34481
43.62288	13.77777	0.80000	0.41224
46.37843	16.53331	0.96000	0.47575
49.13397	19.28885	1.12000	0.53502
51.88953	22.04440	1.28000	0.58994
54.64508	24.79996	1.44000	0.64047
57.40065	27.55553	1.60000	0.68673
60.15620	30.31108	1.76000	0.72887
62.91176	33.06664	1.92000	0.76710
65.66730	35.82217	2.08000	0.80165
68.42285	38.57773	2.24000	0.83277
71.17841	41.33328	2.40000	0.86073
73.93396	44.08884	2.56000	0.88578
76.68951	46.84439	2.72000	0.90816
79.44505	49.59993	2.88000	0.92812
82.20062	52.35550	3.04000	0.94589
84.95618	55.11105	3.20000	0.96168
87.71173	57.86661	3.36000	0.97568
90.46729	60.62216	3.52000	0.98807
93.22284	63.37772	3.68000	0.99904
95.97839	66.13327	3.84000	1.00872
98.73393	68.88881	4.00000	1.01726
98.73393	68.88881	4.00000	1.01725
102.17836	72.33324	4.20000	0.92191
105.62280	75.77768	4.40000	0.82916
109.06725	79.22212	4.60000	0.73939
112.51169	82.66656	4.80000	0.65455
115.95613	86.11101	5.00000	0.57582
119.40056	89.55544	5.20000	0.50376
122.84502	92.99989	5.40000	0.43854
126.28946	96.44434	5.60000	0.38006
129.73390	99.88878	5.80000	0.32800
133.17833	103.33321	6.00000	0.28197
136.62277	106.77765	6.20000	0.24149
140.06721	110.22209	6.40000	0.20606
143.51167	113.66655	6.60000	0.17517
146.95612	117.11099	6.80000	0.14836
150.40054	120.55542	7.00000	0.12514
153.84499	123.99986	7.20000	0.10511
157.28943	127.44431	7.40000	0.08787
160.73387	130.88875	7.60000	0.07306
164.17831	134.33319	7.80000	0.06038
167.62276	137.77763	8.00000	0.04953
171.06720	141.22208	8.20000	0.04027
174.51164	144.66652	8.40000	0.03237
177.95609	148.11096	8.60000	0.02566
181.40053	151.55540	8.80000	0.01996
184.84496	154.99983	9.00000	0.01512

TABLE 29 CONTINUED
m = 3.8

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
32.45564	2.61052	0.16000	0.12623
35.06616	5.22105	0.32000	0.20074
37.67668	7.83157	0.48000	0.27403
40.28722	10.44210	0.64000	0.34491
42.89774	13.05262	0.80000	0.41224
45.50826	15.66314	0.96000	0.47575
48.11877	18.27365	1.12000	0.53502
50.72929	20.88417	1.28000	0.58994
53.33981	23.49469	1.44000	0.64047
55.95035	26.10522	1.60000	0.68673
58.56088	28.71576	1.76000	0.72887
61.17140	31.32628	1.92000	0.76710
63.78192	33.93680	2.08000	0.80165
66.39244	36.54732	2.24000	0.83277
69.00296	39.15784	2.40000	0.86073
71.61349	41.76837	2.56000	0.88578
74.22401	44.37889	2.72000	0.90816
76.83453	46.98941	2.88000	0.92812
79.44507	49.59995	3.04000	0.94589
82.05559	52.21046	3.20000	0.96168
84.66612	54.82100	3.36000	0.97568
87.27664	57.43152	3.52000	0.98807
89.88716	60.04204	3.68000	0.99904
92.49768	62.65256	3.84000	1.00872
95.10820	65.26308	4.00000	1.01726
95.10820	65.26308	4.00000	1.01725
98.37135	68.52623	4.20000	0.92191
101.63451	71.78938	4.40000	0.82916
104.89766	75.05254	4.60000	0.73939
108.16081	78.31569	4.80000	0.65455
111.42397	81.57884	5.00000	0.57582
114.68710	84.84198	5.20000	0.50376
117.95027	88.10515	5.40000	0.43854
121.21342	91.36830	5.60000	0.38006
124.47658	94.63145	5.80000	0.32800
127.73973	97.89461	6.00000	0.28197
131.00288	101.15776	6.20000	0.24149
134.26604	104.42091	6.40000	0.20606
137.52921	107.68408	6.60000	0.17517
140.79236	110.94724	6.80000	0.14836
144.05551	114.21039	7.00000	0.12514
147.31866	117.47354	7.20000	0.10511
150.58182	120.73669	7.40000	0.08787
153.84497	123.99985	7.60000	0.07366
157.10812	127.26300	7.80000	0.06038
160.37129	130.52617	8.00000	0.04953
163.63445	133.78932	8.20000	0.04027
166.89760	137.05247	8.40000	0.03237
170.16075	140.31563	8.60000	0.02566
173.42390	143.57878	8.80000	0.01996
176.68706	146.84193	9.00000	0.01512

TABLE 29 CONTINUED

m = 4.0

TIME	TPRIME	TAU	EFFLUENT CONC.
29.84512	0.00000	0.00000	0.05008
32.32512	2.48000	0.16000	0.12623
34.80511	4.96000	0.32000	0.20074
37.28511	7.44000	0.48000	0.27403
39.76512	9.92000	0.64000	0.34431
42.24512	12.40000	0.80000	0.41224
44.72511	14.88000	0.96000	0.47575
47.20511	17.35999	1.12000	0.53502
49.68510	19.83998	1.28000	0.58994
52.16510	22.31998	1.44000	0.64047
54.64511	24.79999	1.60000	0.68673
57.12511	27.27998	1.76000	0.72887
59.60510	29.75998	1.92000	0.76710
62.08510	32.23997	2.08000	0.80165
64.56509	34.71997	2.24000	0.83277
67.04510	37.19998	2.40000	0.86073
69.52510	39.67998	2.56000	0.88578
72.00510	42.15997	2.72000	0.90816
74.48509	44.63997	2.88000	0.92812
76.96510	47.11998	3.04000	0.94589
79.44510	49.59998	3.20000	0.96168
81.92509	52.07997	3.36000	0.97568
84.40511	54.55998	3.52000	0.98807
86.88510	57.03998	3.68000	0.99904
89.36510	59.51997	3.84000	1.00872
91.84509	61.99997	4.00000	1.01726
94.32509	64.47997	4.16000	1.02475
96.80508	66.95996	4.32000	1.03119
99.28509	69.43997	4.48000	1.03658
101.76508	71.91996	4.64000	1.04093
104.24509	74.39996	4.80000	1.04425
106.72508	76.87995	4.96000	1.04655
109.20507	79.35995	5.12000	1.04782
111.68507	81.83995	5.28000	1.04806
114.16507	84.31995	5.44000	1.04726
116.64508	86.79996	5.60000	1.04542
119.12507	89.27995	5.76000	1.04254
121.60508	91.75995	5.92000	1.03862
124.08507	94.23995	6.08000	1.03366
126.56507	96.71995	6.24000	1.02766
129.04507	99.19995	6.40000	1.02062
131.52508	101.67996	6.56000	1.01254
134.00507	104.15995	6.72000	1.00342
136.48508	106.63995	6.88000	0.99326
138.96508	109.11995	7.04000	0.98206
141.44507	111.59995	7.20000	0.96982
143.92507	114.07995	7.36000	0.95654
146.40507	116.55994	7.52000	0.94222
148.88507	119.03994	7.68000	0.92686
151.36507	121.51995	7.84000	0.91046
153.84508	123.99995	8.00000	0.89302
156.32507	126.47995	8.16000	0.87454
158.80507	128.95995	8.32000	0.85502
161.28507	131.43995	8.48000	0.83446
163.76507	133.91994	8.64000	0.81286
166.24507	136.39995	8.80000	0.79022
168.72507	138.87994	8.96000	0.76654

APPENDIX VII

COMPUTER DEVELOPED STAGED SEQUENCE CYCLIC PROCESS DATA

TABLE 30

EFFECT OF STAGE DURATION TIME ON SEPARATION

NNZ	=	29
H	=	90.0 cm
PHOT	=	0.20
PHOB	=	0.20
BETA	=	1.0
Y_{Ao}	=	0.00095 gmoles/cc
Y_{Bo}	=	0.00086 gmoles/cc
Q	=	25.00 cc

TABLE 30

TIME = 5.00 mins

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.98709	0.85042	1.16170	0.71120	1.00000	1.01457
2	0.94744	0.85973	1.15187	0.70122	0.95748	1.21759
3	0.95509	0.86973	1.21507	0.66767	0.87432	1.57927
4	0.90221	0.80951	1.21558	0.63675	0.82893	1.57668
5	0.88860	0.80801	1.20035	0.62805	0.81161	1.53372
6	0.87575	0.79747	1.19328	0.61726	0.79808	1.53662
7	0.86617	0.79394	1.18625	0.61103	0.78394	1.51174
8	0.85759	0.78727	1.18083	0.60399	0.77386	1.50598
9	0.85075	0.78361	1.17619	0.59874	0.76506	1.49074
10	0.84501	0.77900	1.17249	0.59364	0.75804	1.48337
11	0.84033	0.77579	1.16937	0.58943	0.75216	1.47307
12	0.83644	0.77243	1.16686	0.58560	0.74738	1.46619

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.16261	0.75937	0.98729	1.19735	1.01113	0.83278
2	1.16002	0.72931	0.93831	1.35824	0.98023	0.85061
3	1.14242	0.67729	0.89212	1.42284	0.95441	0.88431
4	1.12690	0.65768	0.88650	1.37416	0.94201	0.88324
5	1.11834	0.65172	0.87067	1.37929	0.92025	0.87180
6	1.10722	0.64338	0.85759	1.35012	0.90898	0.86943
7	1.10039	0.63873	0.84679	1.34429	0.89766	0.86253
8	1.09408	0.63302	0.83763	1.32687	0.88898	0.85939
9	1.08914	0.62905	0.83019	1.31889	0.88151	0.85474
10	1.08495	0.62488	0.82401	1.30731	0.87550	0.85181
11	1.08157	0.62166	0.81895	1.29977	0.87043	0.84848
12	1.07874	0.61853	0.91477	1.29148	0.86630	0.84600

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.99845	1.30271	0.91269	0.84344	1.22853	0.64776
2	1.04724	1.21560	0.89704	0.87044	1.19395	0.69175
3	1.06710	1.18923	0.86734	0.86633	1.15722	0.70236
4	1.03161	1.20026	0.85085	0.84737	1.14947	0.67819
5	1.01882	1.16763	0.83835	0.84726	1.14113	0.67355
6	1.00720	1.16312	0.82387	0.83830	1.13485	0.66081
7	0.99729	1.14446	0.81433	0.83580	1.12905	0.65518
8	0.98929	1.13686	0.80566	0.83021	1.12457	0.64705
9	0.98277	1.12482	0.79882	0.82735	1.12074	0.64181
10	0.97735	1.11739	0.79307	0.82353	1.11769	0.63610
11	0.97293	1.10892	0.78833	0.82095	1.11512	0.63173
12	0.96927	1.10256	0.78441	0.81818	1.11305	0.62752

TABLE 30 CONTINUED

367

TIME = 10.0 mins.

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97743	0.81822	1.21248	0.67323	1.03000	1.01557
2	0.92197	0.86427	1.24188	0.66267	0.91345	1.27908
3	0.87897	0.82979	1.28747	0.61779	0.78748	1.70455
4	0.80623	0.77052	1.28281	0.57204	0.74653	1.74597
5	0.87444	0.75503	1.27437	0.55545	0.73799	1.69730
6	0.86405	0.74971	1.25947	0.54187	0.72470	1.59256
7	0.85601	0.74414	1.26302	0.53140	0.71429	1.64261
8	0.84905	0.73166	1.25908	0.52193	0.70611	1.62729
9	0.84373	0.72576	1.25517	0.51249	0.69926	1.58948
10	0.83925	0.71618	1.25254	0.50489	0.69391	1.57057
11	0.83579	0.71021	1.25013	0.49707	0.68946	1.54176
12	0.83295	0.70281	1.24845	0.49087	0.68596	1.52240

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.21726	0.75215	0.93542	1.25303	1.00599	0.80714
2	1.21715	0.71293	0.87754	1.44456	0.94690	0.83259
3	1.19483	0.63374	0.83821	1.50957	0.88945	0.88647
4	1.17228	0.60339	0.84436	1.46106	0.87379	0.88616
5	1.16416	0.59521	0.82774	1.45825	0.85413	0.87302
6	1.15465	0.58348	0.81783	1.40549	0.84281	0.87044
7	1.14875	0.57775	0.80867	1.39002	0.83132	0.85875
8	1.14295	0.56799	0.80170	1.35088	0.82289	0.85457
9	1.13886	0.56253	0.79585	1.33165	0.81525	0.84538
10	1.13517	0.55467	0.79129	1.30224	0.80970	0.84069
11	1.13246	0.54962	0.78757	1.28260	0.80474	0.83355
12	1.13012	0.54343	0.78461	1.25998	0.80105	0.82887

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.95081	1.36812	0.87633	0.81921	1.29410	0.62538
2	1.02162	1.25576	0.85112	0.85594	1.26375	0.64745
3	1.05621	1.22678	0.81476	0.84871	1.23844	0.62845
4	1.02157	1.23281	0.79898	0.82584	1.23672	0.59245
5	1.01398	1.18203	0.78590	0.82377	1.22943	0.58117
6	1.00240	1.16815	0.77402	0.80981	1.22537	0.56243
7	0.99490	1.13146	0.76557	0.80571	1.22098	0.55192
8	0.98780	1.11392	0.75791	0.79493	1.21820	0.53871
9	0.98277	1.08705	0.75220	0.78994	1.21555	0.52878
10	0.97825	1.06926	0.74723	0.78168	1.21377	0.51887
11	0.97498	1.04898	0.74346	0.77652	1.21220	0.51028
12	0.97216	1.03282	0.74028	0.77011	1.21113	0.50260

TABLE 30 CONTINUED

368

TIME = 15.0

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01599
2	0.91217	0.85041	1.27815	0.64549	0.88999	1.30960
3	0.87290	0.80932	1.33335	0.59426	0.73386	1.79173
4	0.89045	0.75008	1.33478	0.53498	0.70073	1.83100
5	0.28039	0.74103	1.31965	0.51294	0.70753	1.77932
6	0.87224	0.71805	1.31650	0.49637	0.69019	1.76088
7	0.86587	0.71010	1.31116	0.48304	0.68313	1.68042
8	0.86072	0.69090	1.30838	0.47156	0.67664	1.65129
9	0.85691	0.68201	1.30542	0.45881	0.67172	1.58353
10	0.85387	0.66679	1.30381	0.45011	0.66780	1.54860
11	0.85176	0.65749	1.30222	0.43938	0.66482	1.49640
12	0.85012	0.64626	1.30140	0.43238	0.66249	1.46010

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.24946	0.75028	0.89965	1.27831	1.00098	0.79594
2	1.25144	0.70618	0.83986	1.48785	0.92483	0.82491
3	1.22555	0.61011	0.81423	1.54860	0.84210	0.88866
4	1.19612	0.57210	0.83147	1.50043	0.82373	0.88738
5	1.18836	0.56128	0.81383	1.48636	0.80869	0.87355
6	1.18063	0.54726	0.80746	1.40639	0.79737	0.86848
7	1.17526	0.53987	0.80012	1.37855	0.78714	0.85137
8	1.17036	0.52638	0.79531	1.31243	0.77998	0.84507
9	1.16705	0.51965	0.79103	1.27886	0.77330	0.83007
10	1.16404	0.50810	0.78818	1.22884	0.76886	0.82286
11	1.16210	0.50168	0.78573	1.19410	0.76476	0.81086
12	1.16040	0.49267	0.78417	1.15820	0.76209	0.80324

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.91647	1.39661	0.85924	0.80888	1.33311	0.61408
2	1.00022	1.26617	0.82527	0.84983	1.30880	0.62260
3	1.04254	1.23699	0.78734	0.83883	1.29484	0.58427
4	1.00930	1.23590	0.77625	0.81360	1.29706	0.53685
5	1.00669	1.16346	0.76335	0.80782	1.29002	0.52075
6	0.99578	1.13989	0.75442	0.78794	1.28777	0.49679
7	0.99033	1.08219	0.74718	0.78115	1.28452	0.48271
8	0.98446	1.05374	0.74116	0.76397	1.28311	0.46641
9	0.98109	1.01213	0.73677	0.75602	1.28144	0.45295
10	0.97768	0.98337	0.73307	0.74234	1.28077	0.44169
11	0.97583	0.95467	0.73050	0.73383	1.28008	0.43048
12	0.97406	0.92975	0.72840	0.72372	1.27985	0.42234

TABLE 30 CONTINUED

TIME = 20.0

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97166	0.79644	1.26093	0.64951	1.00000	1.01619
2	0.90651	0.34264	1.30313	0.63562	0.87374	1.32771
3	0.37175	0.79621	1.36582	0.57992	0.69587	1.94662
4	0.39742	0.73642	1.36711	0.51074	0.66989	1.88001
5	0.38877	0.72351	1.35040	0.48498	0.68225	1.82598
6	0.32215	0.69398	1.34860	0.46615	0.66868	1.79418
7	0.37712	0.62422	1.34429	0.45120	0.66435	1.68108
8	0.87359	0.65361	1.34239	0.43921	0.65909	1.64172
9	0.87101	0.64786	1.34227	0.42403	0.65576	1.54395
10	0.36920	0.62873	1.33945	0.41591	0.65293	1.49629
11	0.86318	0.61718	1.33853	0.40345	0.65117	1.42799
12	0.86745	0.60533	1.33830	0.39691	0.64971	1.37844

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.27130	0.74933	0.87449	1.29322	0.99680	0.78959
2	1.27459	0.70241	0.81333	1.51467	0.90867	0.82061
3	1.24508	0.59448	0.79929	1.56824	0.80412	0.89022
4	1.20831	0.55037	0.82534	1.52086	0.78365	0.88709
5	1.20058	0.53715	0.80681	1.49664	0.77411	0.87278
6	1.19475	0.52141	0.80347	1.38853	0.76265	0.86487
7	1.18968	0.51278	0.79736	1.35263	0.75448	0.84194
8	1.18577	0.49608	0.79434	1.26077	0.74823	0.83413
9	1.18310	0.48906	0.79125	1.21683	0.74275	0.81311
10	1.18076	0.47451	0.78980	1.15423	0.73937	0.80407
11	1.17947	0.46766	0.78834	1.10855	0.73628	0.78836
12	1.17833	0.45723	0.78779	1.07177	0.73450	0.77847

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.39174	1.41280	0.84865	0.80303	1.35989	0.60676
2	0.98309	1.26725	0.80705	0.84635	1.34063	0.60637
3	1.02954	1.23877	0.76908	0.83155	1.33574	0.55486
4	0.99720	1.23094	0.76299	0.80475	1.34041	0.49808
5	0.99824	1.13622	0.75050	0.79538	1.33300	0.47940
6	0.98820	1.10754	0.74425	0.76928	1.33230	0.45225
7	0.98458	1.03162	0.73801	0.76068	1.32987	0.43666
8	0.97992	0.99658	0.73366	0.73711	1.32951	0.42047
9	0.97813	0.94881	0.73042	0.72717	1.32861	0.40537
10	0.97576	0.91373	0.72796	0.70961	1.32869	0.39584
11	0.97516	0.89715	0.72642	0.69873	1.32864	0.38413
12	0.97433	0.85968	0.72529	0.68798	1.32887	0.37758

TABLE 31

EFFECT OF NUMBER OF CELLS ON SEPARATION

H	=	90.0 cm
PHOT	=	0.200
PHOB	=	0.20
BETA	=	1.0
Y_{Ao}	=	0.00095 gmoles/cc
Y_{Bo}	=	0.00086 gmoles/cc
Q	=	25.00 cc

TABLE 31

NNZ = 9

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97797	0.82237	1.20999	0.68347	1.00000	1.01501
2	0.97433	0.85170	1.20795	0.68809	0.91326	1.25046
3	0.97107	0.88121	1.20460	0.69190	0.76993	1.51027
4	0.89722	0.73722	1.28813	0.55035	0.75278	1.61312
5	0.88815	0.72087	1.27600	0.51613	0.74643	1.52279
6	0.88028	0.69187	1.27315	0.49232	0.73501	1.48389
7	0.87448	0.67720	1.26850	0.47252	0.72604	1.40532
8	0.86942	0.65769	1.26601	0.45859	0.71927	1.36264
9	0.86574	0.64572	1.25340	0.44485	0.71352	1.31020
10	0.86264	0.63325	1.26170	0.43563	0.70919	1.27498
11	0.86031	0.62427	1.26015	0.42667	0.70562	1.24197
12	0.85840	0.61643	1.25905	0.42046	0.70285	1.21596

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.21528	0.75960	0.92653	1.24862	1.00593	0.81094
2	1.21572	0.71846	0.87168	1.41256	0.94946	0.82101
3	1.19604	0.62394	0.83723	1.44552	0.89570	0.85103
4	1.17647	0.57368	0.84677	1.35213	0.88303	0.83839
5	1.17056	0.55405	0.83273	1.31363	0.86642	0.81387
6	1.16310	0.53241	0.82510	1.22852	0.85778	0.80338
7	1.15894	0.52034	0.81796	1.18364	0.84823	0.78430
8	1.15464	0.50511	0.81268	1.12908	0.84212	0.77393
9	1.15180	0.49586	0.80834	1.09090	0.83622	0.76053
10	1.14918	0.48560	0.80503	1.05631	0.83211	0.75203
11	1.14732	0.47879	0.80233	1.02902	0.82847	0.74341
12	1.14572	0.47232	0.80024	1.00723	0.82575	0.73701

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.94149	1.35856	0.88173	0.80930	1.29009	0.63377
2	1.01079	1.23930	0.85740	0.83861	1.26165	0.63894
3	1.04671	1.16872	0.82449	0.81841	1.23929	0.60101
4	1.01604	1.14087	0.81248	0.78112	1.24014	0.54671
5	1.01129	1.05577	0.80202	0.76946	1.23482	0.51669
6	1.00207	1.01319	0.79257	0.74592	1.23249	0.48899
7	0.99666	0.96010	0.78623	0.73393	1.22961	0.46955
8	0.99142	0.92528	0.78037	0.71762	1.22797	0.45372
9	0.98788	0.89352	0.77621	0.70750	1.22636	0.44029
10	0.98474	0.86846	0.77260	0.69699	1.22528	0.43061
11	0.98246	0.84913	0.76991	0.68930	1.22434	0.42200
12	0.98055	0.83275	0.76767	0.68265	1.22364	0.41583

TABLE 31 CONTINUED

NNZ = 19

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97757	0.81922	1.21139	0.67572	1.00000	1.01546
2	0.92267	0.86338	1.24115	0.66337	0.91312	1.27205
3	0.87368	0.85471	1.24471	0.61452	0.76737	1.52112
4	0.88862	0.76063	1.28343	0.56547	0.74705	1.71191
5	0.87729	0.75255	1.27452	0.54359	0.73878	1.65097
6	0.86738	0.73235	1.27003	0.52645	0.72573	1.63568
7	0.85981	0.72412	1.26401	0.51274	0.71547	1.57571
8	0.85326	0.70907	1.26042	0.50112	0.70748	1.55085
9	0.84832	0.70087	1.25683	0.48978	0.70078	1.50602
10	0.84419	0.68969	1.25446	0.48102	0.69559	1.47987
11	0.84106	0.68214	1.25231	0.47215	0.69131	1.44680
12	0.83852	0.67390	1.25082	0.46541	0.68797	1.42266

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.21678	0.75394	0.93299	1.25224	1.00598	0.80801
2	1.21678	0.71415	0.87570	1.43716	0.94740	0.82885
3	1.19501	0.63052	0.83731	1.49397	0.89058	0.87563
4	1.17305	0.59432	0.84437	1.43279	0.87540	0.87175
5	1.16536	0.58266	0.82787	1.41926	0.85626	0.85524
6	1.15625	0.56780	0.81836	1.35570	0.84539	0.85015
7	1.15071	0.55980	0.80957	1.33024	0.83398	0.83609
8	1.14523	0.54800	0.80292	1.28374	0.82622	0.82978
9	1.14142	0.54092	0.79738	1.25700	0.81890	0.81888
10	1.13799	0.53181	0.79311	1.22311	0.81367	0.81259
11	1.13551	0.52573	0.78963	1.19852	0.80901	0.80438
12	1.13338	0.51888	0.78696	1.17372	0.80557	0.79862

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.94830	1.36614	0.87766	0.81536	1.29312	0.62774
2	1.01860	1.25176	0.85257	0.85050	1.26311	0.64495
3	1.05326	1.21152	0.81685	0.83955	1.23836	0.62059
4	1.01939	1.20776	0.80180	0.81249	1.23721	0.57837
5	1.01234	1.14618	0.78917	0.80755	1.23036	0.56177
6	1.00122	1.12299	0.77773	0.79064	1.22670	0.53936
7	0.99415	1.07933	0.76967	0.78395	1.22268	0.52535
8	0.98744	1.05490	0.76235	0.77105	1.22021	0.51024
9	0.98277	1.02408	0.75697	0.76406	1.21785	0.49826
10	0.97861	1.00191	0.75231	0.75446	1.21631	0.48751
11	0.97502	0.97985	0.74881	0.74792	1.21497	0.47801
12	0.97307	0.96153	0.74589	0.74077	1.21405	0.47017

TABLE 31 CONTINUED

NNZ = 39

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97737	0.81772	1.21377	0.67202	1.00500	1.01564
2	0.92153	0.86475	1.24224	0.66212	0.91765	1.29246
3	0.97916	0.83124	1.25787	0.61845	0.72700	1.71501
4	0.83517	0.77551	1.28902	0.57549	0.74649	1.76254
5	0.87311	0.77260	1.27437	0.56169	0.73784	1.72050
6	0.86249	0.75803	1.26921	0.55013	0.72451	1.72135
7	0.85427	0.75457	1.26262	0.54151	0.71406	1.67638
8	0.84715	0.74357	1.25852	0.53329	0.70583	1.66694
9	0.84165	0.73907	1.25446	0.52526	0.69995	1.63344
10	0.83703	0.73060	1.25170	0.51858	0.69353	1.61903
11	0.83344	0.72570	1.24916	0.51165	0.68905	1.59336
12	0.83047	0.71904	1.24738	0.50604	0.68553	1.57741

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.21750	0.75127	0.93665	1.25329	1.00600	0.80671
2	1.21734	0.71235	0.87850	1.44801	0.94668	0.83461
3	1.19477	0.63542	0.83875	1.51703	0.88897	0.89223
4	1.17195	0.60814	0.84463	1.47499	0.87313	0.89376
5	1.16364	0.60181	0.82785	1.47781	0.85325	0.88242
6	1.15395	0.59178	0.81778	1.43093	0.84175	0.88120
7	1.14790	0.58739	0.80848	1.42097	0.82983	0.87085
8	1.14197	0.57884	0.80139	1.38629	0.82155	0.86792
9	1.13775	0.57442	0.79540	1.37162	0.81378	0.85979
10	1.13394	0.56746	0.79073	1.34544	0.80812	0.85612
11	1.13113	0.56319	0.78686	1.32925	0.80304	0.84976
12	1.12870	0.55759	0.78384	1.30880	0.79926	0.84586

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2	
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.95209	1.36904	0.87569	0.82105	1.29458	0.62440
2	1.02320	1.25756	0.85044	0.85888	1.26410	0.64869
3	1.05785	1.23414	0.81378	0.85351	1.23856	0.63244
4	1.02289	1.24525	0.79769	0.83279	1.23658	0.59975
5	1.01506	1.20028	0.78442	0.83223	1.22909	0.59135
6	1.00329	1.19147	0.77236	0.81983	1.22483	0.57483
7	0.99562	1.15897	0.76375	0.81717	1.22027	0.56644
8	0.98835	1.14560	0.75594	0.80764	1.21734	0.55465
9	0.98317	1.12162	0.75010	0.80386	1.21454	0.54622
10	0.97851	1.10694	0.74501	0.79652	1.21265	0.53719
11	0.97511	1.08854	0.74113	0.79230	1.21096	0.52954
12	0.97217	1.07443	0.73784	0.78653	1.20983	0.52235

TABLE 32

EFFECT OF PRODUCT WITHDRAWAL RATE ON SEPARATION

NNZ	=	29
H	=	90.0 cm
BETA	=	1.00
Y_{Ao}	=	0.00095 gmoles/cc
Y_{Bo}	=	0.00086 gmoles/cc
Q	=	25.00 cc

TABLE 32

PHOT = PHOB = 0.10

CONCENTRATION TRANSIENTS IN STAGE 1

T1

T2

T3

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.97569	0.81684	1.21257	0.65912	1.20700	1.21562	1.94956
2	1.71155	0.65571	1.21357	0.62417	1.24235	1.22597	2.64663
3	1.71337	0.65707	1.74757	0.66713	0.84602	1.52846	4.46093
4	1.92341	0.74311	1.74155	0.61537	0.81280	1.54128	4.96722
5	0.93104	0.71781	1.35575	0.49435	0.83165	1.33670	4.40796
6	0.93377	0.67168	1.36071	0.47926	0.83226	1.29536	4.41899
7	0.93674	0.65967	1.36185	0.44459	0.83418	1.18970	4.36858
8	1.93906	0.64023	1.36530	0.43529	0.83602	1.12633	4.22480
9	1.94157	0.62283	1.36687	0.41735	0.83800	1.09643	4.24599
10	1.94415	0.61443	1.36905	0.40709	0.83994	1.02721	4.11206
11	0.94639	0.60298	1.37104	0.39999	0.84191	1.00233	4.08078
12	0.94856	0.59669	1.37275	0.39139	0.84373	0.97323	4.04562

CONCENTRATION TRANSIENTS IN STAGE 2

T2

T3

T1

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.22124	0.71540	0.96991	1.19834	0.99608	0.81199	2.10908
2	1.21230	0.68990	0.92240	1.36450	0.94003	0.87977	2.59947
3	1.12694	0.61498	0.90739	1.33666	0.89833	1.00910	2.84311
4	1.17603	0.59877	0.93471	1.14701	0.90053	0.99722	2.41017
5	1.17811	0.58235	0.93323	1.12347	0.89657	0.93343	2.43544
6	1.17832	0.53647	0.93626	1.03000	0.90156	0.91775	2.41632
7	1.18146	0.52489	0.93775	0.97236	0.90110	0.87566	2.33395
8	1.18266	0.49774	0.94045	0.93750	0.90493	0.85989	2.36862
9	1.18519	0.48551	0.94227	0.88223	0.90677	0.84342	2.28560
10	1.18690	0.47479	0.94468	0.86086	0.90930	0.82319	2.27801
11	1.18883	0.46217	0.94670	0.83462	0.91206	0.81483	2.26775
12	1.19066	0.45650	0.94867	0.81337	0.91424	0.80322	2.23625

CONCENTRATION TRANSIENTS IN STAGE 3

T3

T1

T2

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.98475	1.33629	0.84148	0.86159	1.34914	0.57611	3.17922
2	1.08892	1.16589	0.80654	0.92743	1.32708	0.55935	2.54022
3	1.16031	1.01650	0.77701	0.90918	1.31485	0.53566	2.15039
4	1.14041	1.01936	0.78495	0.83821	1.32385	0.49454	2.39276
5	1.14992	0.94315	0.78561	0.82078	1.32529	0.46979	2.32601
6	1.15042	0.90358	0.78611	0.77673	1.32872	0.45604	2.28843
7	1.15516	0.87747	0.78890	0.76295	1.33084	0.42903	2.35630
8	1.15734	0.83390	0.79046	0.74558	1.33304	0.42072	2.28361
9	1.15995	0.81818	0.79366	0.72661	1.33519	0.40814	2.30749
10	1.16269	0.79781	0.79504	0.71853	1.33691	0.39896	2.29938
11	1.16477	0.78088	0.79712	0.70709	1.33857	0.39373	2.27922
12	1.16707	0.77177	0.79926	0.70016	1.34005	0.38731	2.28802

TABLE 32 CONTINUED
PHOT = PHOB = 0.30

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.97943	0.62110	1.20422	0.68581	1.00000	1.01535	1.78808
2	0.97124	0.70477	1.21494	0.71331	0.89701	1.29340	2.46141
3	0.97021	0.70000	1.23770	0.71071	0.74760	1.67972	3.89855
4	0.96220	0.77472	1.24034	0.70125	0.59672	1.74472	4.73910
5	0.84780	0.78242	1.21192	0.70493	0.67363	1.74268	4.44757
6	0.83158	0.78332	1.20225	0.70634	0.65300	1.77116	4.61662
7	0.81936	0.78777	1.19276	0.71532	0.63642	1.77215	4.64316
8	0.82914	0.78996	1.18597	0.71730	0.62388	1.78671	4.73150
9	0.80115	0.79280	1.18002	0.72451	0.61361	1.78943	4.74963
10	0.79467	0.79449	1.17557	0.72690	0.60565	1.79801	4.80136
11	0.78941	0.79663	1.17171	0.73143	0.59918	1.80118	4.81556
12	0.78517	0.79808	1.16875	0.73351	0.59407	1.80680	4.84599

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.21081	0.79145	0.90751	1.29401	1.00985	0.80513	2.18140
2	1.21329	0.74967	0.84420	1.47314	0.95100	0.80702	2.82422
3	1.19152	0.68623	0.78542	1.58995	0.88768	0.81683	3.51490
4	1.16355	0.66061	0.77437	1.60012	0.86477	0.81914	3.63952
5	1.15091	0.66215	0.74968	1.63824	0.83910	0.81683	3.79829
6	1.13782	0.66514	0.73277	1.63871	0.82273	0.82103	3.82557
7	1.12283	0.66802	0.71880	1.65816	0.80791	0.82319	3.89813
8	1.12095	0.67218	0.70779	1.66095	0.79677	0.82569	3.91341
9	1.11495	0.67435	0.69904	1.67274	0.78743	0.82769	3.95639
10	1.10994	0.67742	0.69202	1.67617	0.78010	0.82940	3.96860
11	1.10600	0.67913	0.68641	1.68367	0.77407	0.83091	3.99460
12	1.10275	0.68128	0.68190	1.68684	0.76927	0.83214	4.02412

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.92290	1.38497	0.90097	0.79497	1.24703	0.70315	2.66144
2	0.96609	1.34253	0.88157	0.81000	1.21780	0.75638	2.23012
3	0.97310	1.39785	0.84326	0.80286	1.18000	0.77681	2.18208
4	0.92976	1.44760	0.81650	0.78970	1.17076	0.77493	2.35225
5	0.91188	1.44686	0.79831	0.79574	1.15843	0.78846	2.33119
6	0.89399	1.47113	0.78206	0.79654	1.15003	0.73987	2.39592
7	0.88070	1.47318	0.77013	0.79995	1.14259	0.80053	2.38746
8	0.86991	1.48301	0.76005	0.80150	1.13700	0.80294	2.42217
9	0.86139	1.49133	0.75220	0.80365	1.13227	0.81008	2.41990
10	0.85453	1.50071	0.74575	0.80499	1.12861	0.81254	2.43932
11	0.84905	1.50407	0.74062	0.80645	1.12555	0.81724	2.43977
12	0.84462	1.51016	0.73644	0.80749	1.12314	0.81940	2.45075

TABLE 32 CONTINUED
PHOT = PHOB = 0.40

CONCENTRATION TRANSIENTS IN STAGE 1

T1 T2 T3

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.97252	0.82565	1.14492	0.89723	1.00000	1.01508	1.73559
2	0.97718	0.84428	1.15407	0.75195	0.98749	1.27944	2.30468
3	0.98110	0.81979	1.17056	0.70009	0.72967	1.62798	3.39001
4	0.98372	0.78078	1.18817	0.79692	0.67768	1.62050	3.71920
5	0.83784	0.78864	1.16804	0.80945	0.64253	1.67738	3.76713
6	0.82021	0.79165	1.15649	0.81203	0.61879	1.69924	3.91099
7	0.80738	0.79485	1.14657	0.82241	0.60003	1.70232	3.95535
8	0.79713	0.79745	1.12937	0.82509	0.58629	1.71152	4.03112
9	0.78931	0.79917	1.13354	0.83050	0.57547	1.71489	4.06728
10	0.78317	0.80071	1.12917	0.83268	0.56726	1.71936	4.11011
11	0.77840	0.80174	1.12566	0.83548	0.56084	1.72175	4.13622
12	0.77466	0.80261	1.12298	0.83698	0.55588	1.72409	4.16138

CONCENTRATION TRANSIENTS IN STAGE 2

T2 T3 T1

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.20245	0.81909	0.89374	1.31250	1.00968	0.80821	2.15585
2	1.20378	0.78399	0.82840	1.47205	0.95158	0.80426	2.72847
3	1.18086	0.73934	0.75734	1.59423	0.88578	0.80352	3.36216
4	1.15057	0.72470	0.73453	1.60508	0.86027	0.80799	3.46929
5	1.13593	0.72819	0.70591	1.63956	0.83370	0.80907	3.62317
6	1.12233	0.73452	0.68576	1.64274	0.81648	0.81209	3.66030
7	1.11286	0.73699	0.67027	1.65718	0.80208	0.81529	3.73333
8	1.10520	0.74140	0.65829	1.66113	0.79129	0.81694	3.76160
9	1.09941	0.74318	0.64915	1.66797	0.78275	0.81885	3.80110
10	1.09484	0.74554	0.64202	1.67109	0.77614	0.81989	3.82235
11	1.09130	0.74675	0.63651	1.67460	0.77094	0.82094	3.84481
12	1.08853	0.74801	0.63220	1.67666	0.76688	0.82159	3.85944

CONCENTRATION TRANSIENTS IN STAGE 3

T3 T1 T2

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.90862	1.38807	0.91367	0.79096	1.21255	0.76613	2.41784
2	0.93372	1.38215	0.89635	0.79751	1.17902	0.82429	2.11726
3	0.92331	1.45582	0.85821	0.79103	1.14067	0.86231	2.08572
4	0.87517	1.50715	0.82805	0.78160	1.12700	0.86714	2.23818
5	0.85111	1.50816	0.80874	0.78653	1.11296	0.88392	2.23115
6	0.83082	1.52995	0.79232	0.78877	1.10315	0.89648	2.29159
7	0.81551	1.53343	0.78040	0.79097	1.09525	0.89556	2.29960
8	0.80389	1.54355	0.77087	0.79276	1.08929	0.89822	2.32855
9	0.79484	1.54708	0.76357	0.79398	1.08459	0.90276	2.33845
10	0.78787	1.55207	0.75783	0.79504	1.08097	0.90481	2.35350
11	0.78243	1.55461	0.75336	0.79575	1.07812	0.90716	2.36136
12	0.77820	1.55722	0.74985	0.79635	1.07591	0.90851	2.36974

TABLE 32 CONTINUED
PHOT = PHOB = 0.50

CONCENTRATION TRANSIENTS IN STAGE 1

N	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.98058	0.83080	1.18587	0.71223	1.00000	1.01463	1.68938
2	0.94750	0.84095	1.18937	0.73046	0.88048	1.24786	2.14348
3	0.91111	0.84720	1.17774	0.73342	0.73730	1.57639	2.95479
4	0.86435	0.77013	1.15007	0.73021	0.67413	1.54347	3.19913
5	0.84731	0.76968	1.14148	0.63019	0.64189	1.52159	3.25930
6	0.83203	0.76784	1.13064	0.62141	0.61983	1.52431	3.38507
7	0.82148	0.76614	1.12222	0.62165	0.60278	1.51957	3.44312
8	0.81344	0.76557	1.11610	0.61873	0.59083	1.51856	3.50373
9	0.80755	0.76482	1.11157	0.61814	0.58182	1.51723	3.54300
10	0.80314	0.76449	1.10820	0.61718	0.57522	1.51647	3.57520
11	0.79985	0.76418	1.10569	0.61673	0.57028	1.51595	3.59869
12	0.79739	0.76400	1.10381	0.61636	0.56661	1.51558	3.61664

CONCENTRATION TRANSIENTS IN STAGE 2

N	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.19391	0.84226	0.88179	1.31783	1.03852	0.81335	2.11848
2	1.19404	0.81201	0.81934	1.44428	0.95517	0.80165	2.59206
3	1.17214	0.77242	0.74524	1.53075	0.89392	0.78813	3.11700
4	1.14344	0.75380	0.71769	1.50965	0.87101	0.78637	3.19077
5	1.12964	0.74746	0.69029	1.51731	0.84820	0.78301	3.32195
6	1.11795	0.74679	0.67098	1.50795	0.83384	0.78028	3.36437
7	1.10992	0.74370	0.65710	1.50754	0.82265	0.77985	3.42397
8	1.10389	0.74325	0.64671	1.50488	0.81450	0.77870	3.45608
9	1.09944	0.74217	0.63912	1.50390	0.80841	0.77834	3.48585
10	1.09613	0.74176	0.63345	1.50298	0.80386	0.77791	3.50625
11	1.09366	0.74136	0.62923	1.50243	0.80045	0.77769	3.52238
12	1.09181	0.74112	0.62608	1.50204	0.79790	0.77751	3.53434

CONCENTRATION TRANSIENTS IN STAGE 3

N	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.89620	1.38258	0.92552	0.78720	1.18599	0.80902	2.26155
2	0.90888	1.38213	0.91092	0.78633	1.15500	0.85478	2.05479
3	0.88963	1.42809	0.87717	0.77424	1.11730	0.87942	2.03948
4	0.84307	1.44706	0.84962	0.76152	1.10296	0.86764	2.18196
5	0.81806	1.42793	0.83313	0.76011	1.09021	0.86970	2.18809
6	0.79932	1.43048	0.81979	0.75900	1.08131	0.86375	2.24039
7	0.78530	1.42512	0.81045	0.75779	1.07470	0.86341	2.25884
8	0.77527	1.42431	0.80338	0.75738	1.06980	0.86156	2.28124
9	0.76773	1.42273	0.79817	0.75687	1.06617	0.86094	2.29492
10	0.76217	1.42200	0.79426	0.75663	1.06346	0.86029	2.30630
11	0.75802	1.42141	0.79134	0.75642	1.06143	0.85993	2.31456
12	0.75491	1.42103	0.78915	0.75629	1.05991	0.85966	2.32085

TABLE 32 CONTINUED
PHOT = PHOB = 0.60

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3		
N	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.99185	0.97641	1.17640	1.72993	1.00000	1.01411	1.63476
2	0.96917	0.94885	1.15447	1.60764	0.87825	1.21953	2.00299
3	0.89962	0.80943	1.14910	0.85839	0.72695	1.44551	2.62981
4	0.87395	0.76979	1.13359	0.85576	0.67649	1.44057	2.82080
5	0.85717	0.76484	1.11606	0.84779	0.64469	1.41356	2.88645
6	0.84406	0.76125	1.10552	0.83523	0.62471	1.40845	2.98398
7	0.83540	0.75830	1.09876	0.83169	0.60982	1.40263	3.03671
8	0.82915	0.75700	1.09272	0.82810	0.59980	1.39938	3.07862
9	0.82475	0.75600	1.08901	0.82626	0.59263	1.39755	3.10906
10	0.82102	0.75545	1.08634	0.82512	0.58757	1.39631	3.12874
11	0.81939	0.75510	1.08445	0.82440	0.58398	1.39561	3.14369
12	0.81779	0.75488	1.08310	0.82398	0.58141	1.39516	3.15423

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1		
N	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.18510	0.86552	0.87155	1.31848	1.00701	0.82030	2.07136
2	1.18311	0.83956	0.81202	1.41515	0.95776	0.80638	2.45588
3	1.16082	0.80448	0.73630	1.47003	0.90024	0.78815	2.88084
4	1.13303	0.78416	0.70524	1.43094	0.87935	0.78268	2.93171
5	1.11940	0.77242	0.67928	1.42450	0.85979	0.77738	3.03908
6	1.10903	0.76847	0.66119	1.41259	0.84774	0.77267	3.08325
7	1.10194	0.76409	0.64896	1.40778	0.83901	0.77102	3.12845
8	1.09698	0.76225	0.64016	1.40436	0.83285	0.76949	3.15715
9	1.09345	0.76088	0.63402	1.40228	0.82850	0.76871	3.17843
10	1.09095	0.76010	0.62964	1.40107	0.82539	0.76820	3.19375
11	1.08916	0.75961	0.62653	1.40029	0.82317	0.76789	3.20461
12	1.08789	0.75931	0.62431	1.39983	0.82159	0.76770	3.21246

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2		
N	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.88521	1.37369	0.93502	0.79089	1.16181	0.84572	2.13182
2	0.88684	1.37232	0.92215	0.78607	1.13327	0.87862	1.99591
3	0.85950	1.39301	0.89203	0.77194	1.09642	0.88992	1.99681
4	0.81462	1.39022	0.86707	0.75911	1.08128	0.86916	2.12308
5	0.78919	1.36450	0.85284	0.75486	1.06951	0.86415	2.13988
6	0.77200	1.35934	0.84203	0.75267	1.06131	0.85675	2.18121
7	0.75940	1.35296	0.83469	0.75076	1.05563	0.85383	2.20270
8	0.75085	1.34976	0.82947	0.74939	1.05155	0.85165	2.21960
9	0.74471	1.34780	0.82575	0.74924	1.04868	0.85037	2.23190
10	0.74057	1.34653	0.82311	0.74888	1.04662	0.84961	2.24046
11	0.73728	1.34580	0.82123	0.74864	1.04516	0.84912	2.24676
12	0.73508	1.34534	0.81988	0.74850	1.04411	0.84893	2.25122

TABLE 32 CONTINUED
PHOT = PHOB = 0.90

CONCENTRATION TRANSIENTS IN STAGE 1

	T1	T2	T3				
N	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.88427	0.85354	1.15231	0.77748	1.01000	1.01262	1.50923
2	0.87127	0.84033	1.13751	0.75332	0.83764	1.15310	1.74707
3	0.82142	0.81609	1.13337	0.90899	0.74646	1.30719	2.12650
4	0.83364	0.78757	1.08720	0.87774	0.70980	1.29526	2.24250
5	0.89032	0.77999	1.07425	0.86367	0.68700	1.26428	2.28900
6	0.88350	0.77671	1.06676	0.85431	0.67541	1.25720	2.32427
7	0.87965	0.77487	1.06258	0.85082	0.66814	1.25386	2.34369
8	0.87737	0.77412	1.05999	0.84912	0.66396	1.25207	2.35437
9	0.87501	0.77376	1.05849	0.84827	0.66150	1.25132	2.36041
10	0.87521	0.77358	1.05760	0.84790	0.66004	1.25095	2.36399
11	0.87473	0.77350	1.05706	0.84772	0.65917	1.25078	2.36607
12	0.87445	0.77346	1.05675	0.84764	0.65866	1.25070	2.36729

CONCENTRATION TRANSIENTS IN STAGE 2

	T2	T3	T1				
N	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.16179	0.90766	0.86073	1.29627	1.00256	0.84160	1.92768
2	1.15476	0.88604	0.91196	1.33981	0.96382	0.82807	2.15051
3	1.13221	0.85326	0.74456	1.34244	0.91770	0.80748	2.39244
4	1.10921	0.83148	0.71551	1.29226	0.90327	0.79751	2.40933
5	1.09791	0.81783	0.69804	1.27778	0.89226	0.79185	2.45743
6	1.09154	0.81296	0.68723	1.27009	0.88615	0.78818	2.48140
7	1.08758	0.81026	0.68120	1.26656	0.88265	0.78683	2.49568
8	1.08532	0.80902	0.67756	1.26501	0.88051	0.78615	2.50464
9	1.08397	0.80847	0.67542	1.26424	0.87927	0.78581	2.50963
10	1.08317	0.80819	0.67416	1.26389	0.87853	0.78566	2.51262
11	1.08269	0.80807	0.67340	1.26372	0.87809	0.78559	2.51438
12	1.08241	0.80801	0.67296	1.26364	0.87783	0.78556	2.51541

CONCENTRATION TRANSIENTS IN STAGE 3

	T3	T1	T2				
N	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.87226	1.33871	0.95109	0.81332	1.11652	0.89271	1.91954
2	0.85895	1.32085	0.94123	0.80535	1.09486	0.89984	1.87133
3	0.82461	1.29615	0.92014	0.79092	1.06446	0.88841	1.88286
4	0.79082	1.27346	0.90381	0.78088	1.05129	0.86511	1.95683
5	0.77174	1.25311	0.89566	0.77616	1.04381	0.85756	1.97640
6	0.76175	1.24655	0.89073	0.77429	1.03909	0.85337	1.99259
7	0.75539	1.24326	0.88780	0.77324	1.03642	0.85146	2.00336
8	0.75177	1.24156	0.88609	0.77278	1.03481	0.85062	2.00911
9	0.74962	1.24084	0.88508	0.77256	1.03386	0.85020	2.01284
10	0.74835	1.24049	0.88447	0.77246	1.03329	0.85011	2.01505
11	0.74759	1.24032	0.88412	0.77241	1.03295	0.84992	2.01637
12	0.74714	1.24024	0.88390	0.77239	1.03275	0.84998	2.01717

TABLE 32 CONTINUED
PHOT = PHOB = 1.0

CONCENTRATION TRANSIENTS IN STAGE 1

T1 T2 T3

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.98498	0.85867	1.14626	0.78523	1.00000	1.01225	1.47765
2	0.95260	0.85251	1.12452	0.85372	0.88570	1.15453	1.69682
3	0.92521	0.82422	1.09295	0.91778	0.75218	1.23863	2.04026
4	0.89784	0.79001	1.07410	0.97525	0.71859	1.24740	2.14231
5	0.89734	0.79001	1.06420	0.87227	0.69811	1.24984	2.18274
6	0.89221	0.78727	1.05748	0.86522	0.68822	1.24377	2.20882
7	0.88917	0.78588	1.05396	0.86242	0.68237	1.24118	2.22290
8	0.88748	0.78533	1.05190	0.86113	0.67916	1.23998	2.22992
9	0.88652	0.78508	1.05075	0.86060	0.67737	1.23936	2.23395
10	0.88592	0.78497	1.05011	0.86036	0.67636	1.23913	2.23612
11	0.88568	0.78492	1.04975	0.86025	0.67579	1.23903	2.23731
12	0.88551	0.78490	1.04955	0.86020	0.67548	1.23898	2.23797

CONCENTRATION TRANSIENTS IN STAGE 2

T2 T3 T1

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.15518	0.91673	0.86017	1.28957	1.00143	0.84791	1.88918
2	1.14658	0.89639	0.81384	1.32500	0.96488	0.83561	2.08248
3	1.12342	0.86522	0.74904	1.32239	0.92117	0.81643	2.29227
4	1.10152	0.84489	0.72116	1.27534	0.90802	0.80679	2.30563
5	1.09079	0.83258	0.70566	1.26209	0.89865	0.80182	2.34322
6	1.08521	0.82835	0.69649	1.25594	0.89361	0.79886	2.36241
7	1.08187	0.82624	0.69162	1.25325	0.89090	0.79781	2.37265
8	1.08007	0.82531	0.68885	1.25214	0.88933	0.79732	2.37881
9	1.07905	0.82493	0.68730	1.25163	0.88846	0.79710	2.38207
10	1.07847	0.82475	0.68644	1.25141	0.88797	0.79700	2.38389
11	1.07815	0.82467	0.68595	1.25132	0.88771	0.79696	2.38492
12	1.07797	0.82464	0.68567	1.25127	0.88754	0.79694	2.38548

CONCENTRATION TRANSIENTS IN STAGE 3

T3 T1 T2

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.87107	1.32939	0.95385	0.82168	1.10582	0.90191	1.87119
2	0.85510	1.30985	0.94439	0.81397	1.08561	0.90545	1.83662
3	0.81998	1.28141	0.92500	0.80066	1.05686	0.89253	1.85046
4	0.78872	1.25932	0.91053	0.79196	1.04435	0.87171	1.91289
5	0.77147	1.24223	0.90352	0.78787	1.03779	0.86514	1.93158
6	0.76299	1.23673	0.89956	0.78634	1.03384	0.86192	1.94419
7	0.75736	1.23425	0.89731	0.78557	1.03171	0.86052	1.95257
8	0.75509	1.23304	0.89607	0.78524	1.03049	0.85994	1.95684
9	0.75353	1.23256	0.89537	0.78510	1.02981	0.85967	1.95943
10	0.75265	1.23234	0.89498	0.78503	1.02943	0.85956	1.96090
11	0.75216	1.23224	0.89475	0.78500	1.02921	0.85951	1.96173
12	0.75188	1.23220	0.89463	0.78499	1.02909	0.85949	1.96221

TABLE 33

EFFECT OF COLUMN DISPLACEMENT VOLUME ON SEPARATION

NNZ	=	29
H	=	90.0 cm
PHOT	=	0.20
PHOB	=	0.20
BETA	=	1.0
Y_{Ao}	=	0.00095 gmoles/cc
Y_{Bo}	=	0.00086 gmoles/cc

TABLE 33

Q = 5.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.99013	0.83630	1.19322	0.89696	1.00000	1.01461	1.73707
2	1.00383	0.83937	1.19067	0.86952	1.08833	0.98953	1.61691
3	1.07284	0.90471	1.18787	0.87435	1.10016	0.95871	1.42550
4	1.04334	0.83529	1.18559	0.89438	1.15126	0.97389	1.44439
5	0.98099	0.85382	1.17643	0.70753	1.10341	1.00641	1.51657
6	0.97598	0.81092	1.17172	0.75492	1.08322	1.01715	1.45744
7	0.94206	0.82568	1.18725	0.72478	1.07024	1.02756	1.57276
8	0.91506	0.83744	1.18329	0.65986	1.06646	1.06605	1.79257
9	0.89901	0.84372	1.16321	0.65461	1.07500	1.06638	1.76270
10	0.89326	0.85957	1.14378	0.66756	1.07389	1.01078	1.61268
11	0.89594	0.87672	1.13037	0.67559	1.05951	0.98313	1.55255
12	0.89442	0.85964	1.12511	0.68628	1.04194	0.98977	1.55733

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.18471	0.64189	1.17810	0.96447	0.98021	0.84205	1.51099
2	1.18867	0.64423	1.14343	0.96953	1.01031	0.84208	1.56448
3	1.16287	0.72312	1.11405	0.98706	1.01472	0.85784	1.42483
4	1.15559	0.72639	1.11150	0.99472	0.95100	0.87464	1.42374
5	1.17745	0.62518	1.09592	1.03542	0.90521	0.88668	1.77942
6	1.15965	0.60942	1.11140	1.06894	0.88706	0.89465	1.84680
7	1.13223	0.62673	1.11608	1.00615	0.87386	0.91425	1.62862
8	1.11453	0.63608	1.10597	0.95251	0.87810	0.94266	1.50907
9	1.10383	0.64366	1.08367	0.95822	0.88436	0.91601	1.51640
10	1.10245	0.66251	1.06467	0.97222	0.87378	0.87185	1.51955
11	1.10476	0.67262	1.05229	0.98104	0.85291	0.86437	1.53128
12	1.10116	0.64783	1.04870	0.99632	0.83290	0.87309	1.61486

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.17666	0.96445	1.02722	0.84242	1.18471	0.64200	1.51255
2	1.14633	0.99045	0.97098	0.86827	1.22109	0.63969	1.64930
3	1.13463	1.06947	0.92618	0.88148	1.23544	0.66569	1.74930
4	1.18058	1.02433	0.91609	0.88039	1.19243	0.69644	1.48558
5	1.19635	0.91719	0.89824	0.93001	1.16861	0.70532	1.27024
6	1.16346	0.92205	0.91382	0.92411	1.15656	0.71192	1.28746
7	1.13280	0.94252	0.91988	0.85621	1.14907	0.74063	1.29087
8	1.11437	0.95195	0.89951	0.83780	1.15596	0.75995	1.29940
9	1.10381	0.96600	0.87368	0.84909	1.15817	0.71887	1.40995
10	1.10614	0.99125	0.85436	0.85802	1.14671	0.68162	1.50758
11	1.10878	0.98807	0.84396	0.86664	1.12973	0.68166	1.47690
12	1.10044	0.95092	0.84284	0.88236	1.11503	0.69122	1.39394

TABLE 33 CONTINUED

Q = 10.00 cc.

CONCENTRATION TRANSIENTS IN STAGE 1							
	T1		T2		T3		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.97305	0.82454	1.20857	0.67982	1.00000	1.01505	1.80455
2	0.94431	0.89815	1.14447	0.71709	1.15507	0.98028	1.35443
3	0.90100	0.90560	1.07021	0.75000	1.23725	0.93500	1.10414
4	0.85700	0.86007	1.07571	0.81539	1.19116	1.04249	1.15474
5	0.81172	0.84615	1.08700	0.78111	1.18456	1.08164	1.27071
6	0.99689	0.87387	1.07513	0.72637	1.18325	1.07847	1.34907
7	0.98704	0.89163	1.06208	0.75174	1.17829	1.02741	1.23192
8	0.98556	0.86632	1.05347	0.77566	1.16533	1.04113	1.20162
9	0.97267	0.84791	1.05174	0.76445	1.15628	1.05331	1.25328
10	0.96082	0.85975	1.04561	0.73854	1.15317	1.05544	1.29580
11	0.95510	0.87038	1.03763	0.74176	1.14680	1.03478	1.26225
12	0.94927	0.86206	1.03245	0.75512	1.13846	1.02883	1.23559

CONCENTRATION TRANSIENTS IN STAGE 2							
	T2		T3		T1		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.20027	0.63539	1.17913	0.97318	0.97807	0.82937	1.55908
2	1.14120	0.74573	1.20301	0.98356	0.99427	0.83855	1.25114
3	1.09319	0.74893	1.19268	1.05008	1.00288	0.85606	1.28515
4	1.09877	0.65663	1.18251	1.07957	0.97453	0.88750	1.52769
5	1.08549	0.67456	1.19658	1.02215	0.96101	0.91472	1.37461
6	1.07509	0.70410	1.17939	0.99953	0.96417	0.88454	1.29404
7	1.07267	0.71277	1.16661	1.02678	0.95292	0.85511	1.52456
8	1.07010	0.67982	1.16130	1.04388	0.93930	0.87166	1.41493
9	1.06315	0.67010	1.15794	1.02334	0.93203	0.88698	1.40212
10	1.05703	0.68553	1.14894	1.00502	0.92794	0.87709	1.34879
11	1.05371	0.69242	1.14065	1.01394	0.91962	0.86078	1.35273
12	1.05013	0.68006	1.13602	1.02438	0.91115	0.86365	1.39242

CONCENTRATION TRANSIENTS IN STAGE 3							
	T3		T1		T2		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.18696	1.00209	0.89769	0.87685	1.21183	0.63318	1.61579
2	1.14366	1.06958	0.92876	0.85684	1.14493	0.69584	1.53881
3	1.10309	1.03464	0.92312	0.89417	1.08149	0.75220	1.34854
4	1.10293	0.95333	0.90350	0.88729	1.06946	0.79133	1.16817
5	1.08475	0.98863	0.91287	0.82769	1.05932	0.81013	1.19173
6	1.07229	1.01758	0.89382	0.83957	1.06249	0.76127	1.32448
7	1.07293	1.00573	0.88079	0.86165	1.05438	0.74575	1.32530
8	1.06517	0.97313	0.87779	0.86223	1.04553	0.76787	1.24395
9	1.05418	0.97670	0.87192	0.83901	1.04183	0.78000	1.25752
10	1.04739	0.99329	0.86195	0.83474	1.03896	0.76262	1.29198
11	1.04352	0.99166	0.85435	0.84579	1.03366	0.74883	1.31175
12	1.03693	0.97643	0.84996	0.84855	1.02842	0.75617	1.28063

TABLE 33 CONTINUED

Q = 15.00 cc

CONCENTRATION TRANSIENTS IN STAGE 1							
	T1		T2		T3		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.97738	0.82102	1.21336	0.67438	1.00700	1.01544	1.82701
2	0.89656	0.93992	1.21420	0.65613	1.08526	1.00767	1.71836
3	0.87170	0.73204	1.15000	0.70414	1.14339	0.90070	1.45844
4	0.75243	0.82147	1.13131	0.70029	1.13587	1.01414	1.44309
5	0.83443	0.86139	1.08220	0.64313	1.13386	0.99188	1.47213
6	0.81748	0.85923	1.05586	0.67040	1.08198	0.95471	1.38971
7	0.79817	0.83271	1.04957	0.66776	1.04810	0.97743	1.46579
8	0.77153	0.84230	1.02900	0.64933	1.03311	0.96538	1.47956
9	0.75762	0.84363	1.00937	0.65590	1.00728	0.95124	1.45329
10	0.74222	0.83205	0.99746	0.65669	0.98608	0.95801	1.47569
11	0.72552	0.83371	0.98313	0.64825	0.97093	0.95400	1.49116
12	0.71422	0.83532	0.97016	0.64932	0.95374	0.94675	1.48238

CONCENTRATION TRANSIENTS IN STAGE 2							
	T2		T3		T1		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.20910	0.64997	1.09676	1.02069	0.97738	0.82420	1.73121
2	1.17401	0.70197	1.11358	1.01357	0.86010	0.94742	1.52223
3	1.07924	0.67438	1.17986	1.01336	0.71250	1.11120	1.37349
4	0.98989	0.61544	1.18633	0.97183	0.72418	1.11740	1.31761
5	0.97207	0.63465	1.10961	0.95212	0.73741	1.06262	1.31427
6	0.97156	0.61634	1.08020	0.97204	0.68140	1.07066	1.41850
7	0.94359	0.60727	1.06553	0.94483	0.65213	1.08414	1.37774
8	0.92431	0.61584	1.03110	0.93849	0.63493	1.05533	1.36610
9	0.91211	0.60779	1.00988	0.94786	0.60797	1.05428	1.40853
10	0.89577	0.60244	0.99205	0.93597	0.59043	1.06217	1.40284
11	0.88353	0.60556	0.97045	0.93081	0.57529	1.04920	1.39942
12	0.87324	0.60246	0.95478	0.93468	0.55861	1.04604	1.41895

CONCENTRATION TRANSIENTS IN STAGE 3							
	T3		T1		T2		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.11210	1.16756	0.79443	0.97979	1.28652	0.61243	2.20545
2	1.20070	1.10150	0.76517	1.06990	1.23906	0.65270	1.74151
3	1.23419	1.05414	0.79382	1.07802	1.16397	0.73713	1.34869
4	1.14657	1.11253	0.81516	1.00544	1.13715	0.73928	1.49253
5	1.12399	1.12143	0.75418	1.04352	1.11433	0.69442	1.60102
6	1.10700	1.07477	0.72998	1.04874	1.08157	0.71017	1.47783
7	1.06571	1.08170	0.71151	1.01697	1.06859	0.71555	1.51580
8	1.04510	1.09275	0.68195	1.02291	1.05111	0.69583	1.57946
9	1.02406	1.07005	0.66576	1.02900	1.02992	0.69814	1.54147
10	0.99795	1.06906	0.64931	1.01426	1.01667	0.70243	1.55048
11	0.98085	1.07537	0.63080	1.01397	1.00244	0.69343	1.58493
12	0.96356	1.06529	0.61795	1.01762	0.98800	0.69267	1.57695

TABLE 33 CONTINUED

Q = 20.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.97554	0.81637	1.21977	0.66898	1.00000	1.01556	1.85171
2	0.95277	0.90564	1.26369	0.62873	0.97512	1.13109	2.43447
3	0.93011	0.87039	1.32265	0.60517	0.95305	1.47262	3.58278
4	0.92342	0.77131	1.74337	0.57933	0.92135	1.45033	3.64995
5	0.93365	0.76722	1.34088	0.56136	0.97111	1.28726	3.16349
6	0.94934	0.73647	1.35382	0.55997	0.97113	1.30166	3.24052
7	0.96160	0.73166	1.36288	0.52801	0.99251	1.26780	3.29712
8	0.97323	0.72612	1.37010	0.52657	1.00234	1.21705	3.15772
9	0.98320	0.71007	1.37783	0.51906	1.01463	1.21467	3.17781
10	0.99223	0.70818	1.38352	0.50911	1.02515	1.18283	3.13555
11	1.00006	0.70193	1.38919	0.50751	1.03374	1.16944	3.09661
12	1.00701	0.69686	1.39385	0.50149	1.04242	1.16173	3.09753

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.22137	0.70031	1.00278	1.14974	0.98554	0.81567	1.99962
2	1.20407	0.69528	0.96562	1.29005	0.90250	0.93402	2.31360
3	1.16481	0.65073	1.01740	1.27816	0.81411	1.14338	2.24879
4	1.14082	0.65571	1.07879	1.12629	0.83986	1.13913	1.81641
5	1.15262	0.65016	1.07270	1.16034	0.86667	1.05070	1.91767
6	1.16648	0.60028	1.09893	1.12830	0.87824	1.05987	1.99518
7	1.17337	0.60283	1.10877	1.07679	0.89809	1.03625	1.89014
8	1.18322	0.58948	1.12180	1.07687	0.91013	1.02020	1.92686
9	1.18997	0.57783	1.13305	1.04575	0.92380	1.01820	1.93071
10	1.19680	0.57611	1.14203	1.03372	0.93429	1.00078	1.88037
11	1.20247	0.56642	1.15131	1.02690	0.94423	0.99662	1.89353
12	1.20756	0.56315	1.15854	1.01193	0.95302	0.99174	1.87293

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.01812	1.30680	0.81242	0.91782	1.34245	0.58961	2.92241
2	1.13040	1.15649	0.76822	1.01063	1.32013	0.58402	2.31260
3	1.20409	1.03316	0.76434	1.00293	1.31528	0.60441	1.86723
4	1.19234	1.09405	0.79114	0.91290	1.33582	0.58728	2.08708
5	1.22267	1.06724	0.79507	0.91871	1.34173	0.55792	2.09918
6	1.23095	1.02074	0.81544	0.89301	1.35066	0.55821	2.00429
7	1.24433	1.02226	0.82485	0.88204	1.35883	0.53744	2.07711
8	1.25577	0.99485	0.83687	0.87907	1.36464	0.53279	2.02914
9	1.26443	0.98528	0.84640	0.86250	1.37087	0.52852	2.02117
10	1.27375	0.97965	0.85495	0.85957	1.37569	0.51955	2.03650
11	1.28075	0.96627	0.86281	0.85439	1.38021	0.51773	2.01132
12	1.28735	0.96286	0.86945	0.84834	1.38416	0.51370	2.01498

TABLE 33 CONTINUED
Q = 30.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.97887	0.82282	1.20054	0.68893	1.00000	1.01493	1.76863
2	0.93681	0.94097	1.21613	0.72154	0.89903	1.24622	2.33637
3	0.99302	0.79776	1.24137	0.70534	0.76862	1.55074	3.54140
4	0.91918	0.77167	1.24147	0.57049	0.72660	1.53075	3.97529
5	0.87790	0.71493	1.32647	0.64672	0.70806	1.51326	4.05306
6	0.86527	0.71341	1.22008	0.61936	0.69253	1.50403	4.27824
7	0.85613	0.70471	1.21280	0.60633	0.67768	1.47830	4.36335
8	0.84769	0.69745	1.20750	0.58879	0.66671	1.46474	4.50553
9	0.84101	0.69089	1.20276	0.57879	0.65692	1.44749	4.57894
10	0.83526	0.68557	1.19899	0.56703	0.64906	1.43562	4.67695
11	0.83052	0.68073	1.19572	0.55914	0.64235	1.42314	4.73787
12	0.82651	0.67670	1.19306	0.55093	0.63681	1.41356	4.80704

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.20752	0.80308	0.89954	1.29437	1.01657	0.80329	2.16360
2	1.21301	0.75023	0.84328	1.43925	0.96975	0.78758	2.75954
3	1.19703	0.66813	0.79357	1.50293	0.92553	0.76474	3.39311
4	1.17528	0.62030	0.79002	1.45606	0.91147	0.75053	3.49201
5	1.16708	0.60114	0.77217	1.44815	0.89092	0.73569	3.64105
6	1.15641	0.58816	0.75845	1.41165	0.87965	0.72661	3.65949
7	1.14966	0.57538	0.74696	1.39483	0.86784	0.71995	3.73112
8	1.14313	0.56761	0.73718	1.37047	0.85894	0.71327	3.74408
9	1.13806	0.55882	0.72919	1.35518	0.85108	0.70856	3.78484
10	1.13364	0.55294	0.72244	1.33794	0.84464	0.70380	3.79695
11	1.13002	0.54680	0.71683	1.32540	0.83915	0.70022	3.82111
12	1.12694	0.54225	0.71212	1.31270	0.83457	0.69679	3.83096

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.91517	1.37934	0.91897	0.77712	1.24674	0.70083	2.68122
2	0.95600	1.32315	0.90709	0.77762	1.21542	0.75291	2.23429
3	0.96742	1.33530	0.87785	0.75350	1.18625	0.75144	2.17896
4	0.93265	1.33690	0.85731	0.72602	1.18208	0.71302	2.37645
5	0.91987	1.28765	0.84499	0.71900	1.17322	0.69712	2.35580
6	0.90608	1.27080	0.83161	0.71086	1.16718	0.66969	2.44441
7	0.89483	1.23872	0.82235	0.70466	1.16152	0.65645	2.44940
8	0.88566	1.22166	0.81377	0.69952	1.15711	0.63854	2.49961
9	0.87786	1.19973	0.80694	0.69485	1.15328	0.62766	2.51111
10	0.87142	1.18522	0.80107	0.69105	1.15018	0.61537	2.54215
11	0.86600	1.16947	0.79621	0.68760	1.14753	0.60673	2.55412
12	0.86147	1.15777	0.79209	0.68473	1.14537	0.59797	2.57424

TABLE 33 CONTINUED
Q = 35.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.98038	0.82974	1.18767	0.70919	1.00000	1.01374	1.69769
2	0.94895	0.83040	1.19589	0.75973	0.90774	1.17731	2.05045
3	0.91309	0.77660	1.01364	0.75706	0.73957	1.34806	2.73707
4	0.90343	0.70519	1.01794	0.69356	0.75695	1.30578	3.01776
5	0.90170	0.68077	1.00262	0.64711	0.73910	1.23771	3.11216
6	0.89235	0.66248	1.19822	0.59877	0.72842	1.20524	3.31111
7	0.88637	0.54635	1.19358	0.57091	0.71672	1.17616	3.43054
8	0.88030	0.63551	1.18973	0.54583	0.70872	1.15296	3.54587
9	0.87659	0.62671	1.18672	0.52933	0.70173	1.13540	3.63394
10	0.87277	0.61951	1.18414	0.51430	0.69610	1.12094	3.70761
11	0.86978	0.61405	1.18205	0.50365	0.69152	1.10974	3.76640
12	0.86734	0.60993	1.18032	0.49530	0.68775	1.10071	3.81391

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.19561	0.83795	0.88287	1.28596	1.02064	0.80674	2.07826
2	1.20295	0.77935	0.83676	1.36713	0.98431	0.77805	2.52190
3	1.19287	0.68951	0.79115	1.36802	0.95247	0.72992	2.99148
4	1.17531	0.62840	0.78631	1.27215	0.94504	0.70005	3.02594
5	1.17030	0.58931	0.77393	1.22855	0.92999	0.67687	3.15244
6	1.16292	0.56467	0.76277	1.18242	0.92288	0.65680	3.19251
7	1.15824	0.54213	0.75448	1.14958	0.91563	0.64452	3.25526
8	1.15414	0.52756	0.74715	1.12280	0.90991	0.63355	3.28757
9	1.15075	0.51522	0.74138	1.10153	0.90532	0.62591	3.31849
10	1.14801	0.50624	0.73662	1.08476	0.90146	0.61967	3.33953
11	1.14573	0.49907	0.73272	1.07132	0.89834	0.61496	3.35662
12	1.14387	0.49357	0.72954	1.06072	0.89575	0.61123	3.36956

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.89806	1.35804	0.94662	0.75479	1.21391	0.75001	2.44750
2	0.92427	1.30231	0.94266	0.74815	1.18721	0.78660	2.12660
3	0.93036	1.25892	0.92305	0.71057	1.16117	0.76435	2.05566
4	0.90305	1.21432	0.90605	0.67637	1.15872	0.69317	2.24785
5	0.89181	1.13989	0.89865	0.65795	1.15292	0.65443	2.25180
6	0.88203	1.09928	0.88945	0.64525	1.14831	0.61502	2.32700
7	0.87291	1.06046	0.88338	0.63400	1.14461	0.58931	2.35959
8	0.86629	1.03177	0.87806	0.62645	1.14142	0.56769	2.39469
9	0.86053	1.00842	0.87373	0.62008	1.13885	0.55159	2.41949
10	0.85592	0.98993	0.87022	0.61537	1.13672	0.53886	2.43979
11	0.85214	0.97528	0.86730	0.61160	1.13496	0.52897	2.45567
12	0.84903	0.96361	0.86492	0.60869	1.13351	0.52124	2.46816

TABLE 33 CONTINUED

Q = 40.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

N	T1		T2		T3		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.98134	0.83773	1.17480	0.73234	1.00000	1.01261	1.62331
2	0.95715	0.82900	1.17630	0.79503	0.95771	1.14112	1.86019
3	0.92308	0.77674	1.18374	0.80415	0.80718	1.25120	2.29315
4	0.91413	0.71039	1.18198	0.73094	0.77444	1.19766	2.50001
5	0.90719	0.88442	1.17055	0.89002	0.75383	1.14090	2.60519
6	0.89746	0.66585	1.16438	0.63234	0.74285	1.10714	2.74220
7	0.89094	0.65043	1.15931	0.60384	0.73112	1.08337	2.84488
8	0.88527	0.64022	1.15452	0.58171	0.72257	1.06420	2.92304
9	0.88030	0.63246	1.15091	0.56557	0.71553	1.05031	2.98855
10	0.87670	0.62674	1.14780	0.55391	0.70972	1.04077	3.03873
11	0.87351	0.62254	1.14523	0.54520	0.70502	1.03324	3.07845
12	0.87089	0.61940	1.14311	0.53879	0.70113	1.02764	3.10962

CONCENTRATION TRANSIENTS IN STAGE 2

N	T2		T3		T1		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.18345	0.86887	0.87492	1.27136	1.02204	0.81493	1.97923
2	1.18987	0.80965	0.83560	1.31538	0.98917	0.79008	2.31341
3	1.18042	0.72244	0.79059	1.29178	0.95883	0.74152	2.66972
4	1.16127	0.66417	0.78020	1.19583	0.95154	0.70732	2.68151
5	1.15549	0.62031	0.76790	1.14684	0.93712	0.68287	2.78200
6	1.14811	0.59323	0.75567	1.10918	0.92915	0.66154	2.84075
7	1.14239	0.57105	0.74684	1.08090	0.92226	0.64822	2.89532
8	1.13797	0.55605	0.73916	1.06071	0.91624	0.63792	2.93680
9	1.13410	0.54496	0.73294	1.04528	0.91161	0.63046	2.96788
10	1.13099	0.53678	0.72790	1.03387	0.90767	0.62502	2.99266
11	1.12841	0.53081	0.72373	1.02533	0.90445	0.62095	3.01176
12	1.12626	0.52635	0.72031	1.01893	0.90180	0.61795	3.02681

CONCENTRATION TRANSIENTS IN STAGE 3

N	T3		T1		T2		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.88891	1.33386	0.96295	0.77514	1.18440	0.79653	2.23127
2	0.90302	1.28156	0.96166	0.75236	1.16081	0.81826	2.01333
3	0.90140	1.21471	0.94518	0.71292	1.13451	0.78724	1.94202
4	0.87565	1.15905	0.92694	0.68162	1.12932	0.71263	2.09764
5	0.86165	1.09563	0.91893	0.66019	1.12317	0.67078	2.12912
6	0.85161	1.05741	0.91008	0.64669	1.11724	0.63677	2.17854
7	0.84160	1.02810	0.90346	0.63564	1.11285	0.61297	2.21783
8	0.83435	1.00554	0.89817	0.62812	1.10897	0.59564	2.24381
9	0.82820	0.98927	0.89365	0.62251	1.10579	0.58267	2.26691
10	0.82313	0.97685	0.89002	0.61836	1.10317	0.57318	2.28406
11	0.81903	0.96760	0.88700	0.61532	1.10098	0.56610	2.29763
12	0.81583	0.96066	0.88451	0.61304	1.09916	0.56083	2.30837

TABLE 33 CONTINUED

Q = 45.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.98316	0.84599	1.15288	0.75534	1.00000	1.01140	1.55712
2	0.96792	0.83115	1.16074	0.82023	0.91494	1.11274	1.72106
3	0.97477	0.78119	1.16015	0.87152	0.92226	1.18363	2.01148
4	0.92407	0.72357	1.16017	0.75033	0.79959	1.12661	2.17858
5	0.91841	0.69230	1.15017	0.89671	0.78033	1.07901	2.26361
6	0.91003	0.67310	1.14384	0.65377	0.77053	1.04578	2.37460
7	0.90428	0.65893	1.13941	0.62551	0.76093	1.02398	2.45128
8	0.89965	0.64928	1.13500	0.60593	0.75356	1.00772	2.50495
9	0.89564	0.64252	1.13170	0.59187	0.74795	0.99645	2.54735
10	0.89253	0.63768	1.12892	0.58209	0.74321	0.98849	2.57965
11	0.88996	0.63426	1.12671	0.57513	0.73946	0.98277	2.60365
12	0.88737	0.63182	1.12488	0.57018	0.73643	0.97871	2.62193

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.17186	0.89222	0.87234	1.24704	1.02183	0.82518	1.87758
2	1.17738	0.83301	0.84077	1.26456	0.99283	0.80383	2.12585
3	1.16958	0.74573	0.80096	1.22487	0.96533	0.75702	2.39843
4	1.15226	0.68911	0.78922	1.13645	0.95951	0.71811	2.43777
5	1.14554	0.64414	0.77920	1.08644	0.94739	0.69223	2.47963
6	1.13942	0.61552	0.76845	1.05340	0.94008	0.67172	2.53761
7	1.13398	0.59468	0.76084	1.02941	0.93460	0.65817	2.57999
8	1.13010	0.58024	0.75452	1.01278	0.92951	0.64868	2.61430
9	1.12674	0.57025	0.74931	1.00091	0.92571	0.64187	2.63933
10	1.12402	0.56313	0.74521	0.99240	0.92257	0.63712	2.65812
11	1.12183	0.55810	0.74187	0.98635	0.91999	0.63373	2.67252
12	1.12002	0.55453	0.73916	0.98201	0.91793	0.63131	2.68338

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.88508	1.30433	0.97468	0.78917	1.16253	0.82693	2.07174
2	0.89263	1.25070	0.97497	0.76323	1.14303	0.83325	1.92204
3	0.88881	1.16799	0.96220	0.72192	1.11907	0.79294	1.85459
4	0.86731	1.10778	0.94525	0.69232	1.11293	0.72079	1.97213
5	0.85384	1.05514	0.93785	0.66987	1.10780	0.67800	2.01912
6	0.84544	1.02006	0.93073	0.65552	1.10214	0.64818	2.05158
7	0.83678	0.99589	0.92486	0.64504	1.09813	0.62713	2.08398
8	0.83052	0.97798	0.92054	0.63776	1.09472	0.61259	2.10433
9	0.82547	0.96546	0.91684	0.63269	1.09187	0.60221	2.12057
10	0.82127	0.95649	0.91388	0.62906	1.08959	0.59484	2.13333
11	0.81795	0.95004	0.91149	0.62649	1.08771	0.58961	2.14271
12	0.81524	0.94545	0.90954	0.62466	1.08617	0.58587	2.15003

TABLE 33 CONTINUED

Q = 50.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

	T1	T2	T3	T4	T5	T6	T7
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.98427	0.85354	1.15281	0.77348	1.00000	1.01048	1.50603
2	0.96854	0.83552	1.14836	0.83799	0.92141	1.09798	1.63297
3	0.94215	0.79686	1.14584	0.85097	0.83768	1.15154	1.85104
4	0.91778	0.75843	1.14331	0.78879	0.81264	1.09555	1.98951
5	0.89335	0.70545	1.13422	0.71645	0.79991	1.05453	2.08704
6	0.91778	0.68649	1.12772	0.67809	0.79090	1.02342	2.15204
7	0.91238	0.67345	1.12356	0.65161	0.78263	1.00295	2.20969
8	0.90835	0.66447	1.11940	0.63394	0.77529	0.93864	2.24997
9	0.90472	0.65937	1.11627	0.62161	0.77100	0.97865	2.27947
10	0.90197	0.65412	1.11378	0.61308	0.76691	0.97182	2.30210
11	0.89976	0.65117	1.11169	0.60720	0.76367	0.96705	2.31844
12	0.89795	0.64912	1.11004	0.60311	0.76111	0.96374	2.33051

CONCENTRATION TRANSIENTS IN STAGE 2

	T2	T3	T4	T5	T6	T7	T8
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.16179	0.90766	0.87401	1.22685	1.02117	0.83476	1.79671
2	1.16633	0.85023	0.84785	1.23099	0.99444	0.81671	1.99167
3	1.15935	0.76509	0.81209	1.18683	0.96825	0.77326	2.21456
4	1.14276	0.71160	0.79941	1.10887	0.96293	0.73295	2.22759
5	1.13549	0.66870	0.79060	1.06149	0.95219	0.70698	2.27986
6	1.13004	0.64025	0.78082	1.03153	0.94512	0.68800	2.33172
7	1.12475	0.62086	0.77388	1.01078	0.94032	0.67491	2.36618
8	1.12108	0.60737	0.76837	0.99644	0.93576	0.66611	2.39371
9	1.11932	0.59820	0.76376	0.98658	0.93236	0.65995	2.41421
10	1.11550	0.59186	0.76021	0.97968	0.92965	0.65569	2.42885
11	1.11352	0.58746	0.75734	0.97487	0.92741	0.65275	2.43992
12	1.11191	0.58441	0.75504	0.97153	0.92564	0.65069	2.44812

CONCENTRATION TRANSIENTS IN STAGE 3

	T3	T4	T5	T6	T7	T8	T9
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.88568	1.28076	0.98144	0.80328	1.14652	0.84717	1.95704
2	0.88948	1.22886	0.98218	0.77647	1.12991	0.84441	1.84864
3	0.88439	1.14319	0.97147	0.73489	1.10766	0.80125	1.78694
4	0.86963	1.08433	0.95539	0.70702	1.10056	0.73556	1.87422
5	0.85259	1.03993	0.94795	0.68522	1.09591	0.69448	1.92474
6	0.84506	1.00833	0.94181	0.67075	1.09047	0.66763	1.94892
7	0.83733	0.98733	0.93633	0.66086	1.08661	0.64901	1.97419
8	0.83164	0.97245	0.93245	0.65396	1.08349	0.63629	1.99115
9	0.82724	0.96209	0.92922	0.64925	1.08084	0.62752	2.00319
10	0.82356	0.95494	0.92660	0.64599	1.07877	0.62141	2.01293
11	0.82070	0.94992	0.92454	0.64372	1.07708	0.61717	2.01999
12	0.81840	0.94643	0.92287	0.64214	1.07571	0.61422	2.02532

TABLE 33 CONTINUED

Q = 60.0 cc

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.98618	0.86779	1.13504	0.80577	0.99999	1.00685	1.42112
2	0.97543	0.84623	1.12309	0.86680	0.93242	1.07948	1.50670
3	0.95394	0.80253	1.12099	0.88291	0.86234	1.11606	1.64322
4	0.93151	0.76071	1.11707	0.89721	0.84903	1.06432	1.73594
5	0.93754	0.73501	1.11032	0.75937	0.83276	1.03209	1.81215
6	0.93151	0.71750	1.10412	0.72864	0.82452	1.00630	1.84938
7	0.92690	0.70636	1.10054	0.70599	0.81848	0.98820	1.88209
8	0.92378	0.69859	1.09707	0.69126	0.81305	0.97655	1.90623
9	0.92102	0.69346	1.09438	0.68148	0.80927	0.96844	1.92173
10	0.91890	0.69003	1.09238	0.67473	0.80629	0.96296	1.93355
11	0.91728	0.68768	1.09072	0.67023	0.80389	0.95930	1.94200
12	0.91597	0.68611	1.08942	0.66720	0.80206	0.95681	1.94788

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.14384	0.93156	0.87996	1.19072	1.01882	0.85333	1.66151
2	1.14659	0.87981	0.86221	1.17992	0.99599	0.84032	1.78346
3	1.14104	0.80086	0.83405	1.13525	0.97239	0.80400	1.93929
4	1.12638	0.75385	0.82105	1.07701	0.96780	0.76492	1.95996
5	1.11841	0.71763	0.81426	1.03716	0.95948	0.74025	1.98511
6	1.11413	0.69115	0.80655	1.01222	0.95319	0.72430	2.02303
7	1.10947	0.67432	0.80089	0.99609	0.94945	0.71259	2.04634
8	1.10623	0.66279	0.79678	0.98494	0.94591	0.70496	2.06320
9	1.10378	0.65492	0.79332	0.97752	0.94321	0.69988	2.07670
10	1.10171	0.64971	0.79068	0.97254	0.94120	0.69637	2.08572
11	1.10014	0.64618	0.78864	0.96915	0.93955	0.69402	2.09220
12	1.09890	0.64379	0.78702	0.96686	0.93826	0.69244	2.09697

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.82964	1.23850	0.99002	0.82986	1.12192	0.87891	1.77706
2	0.88927	1.19320	0.99079	0.80381	1.11020	0.86497	1.72217
3	0.88329	1.11329	0.98316	0.76325	1.09163	0.82158	1.67465
4	0.86913	1.06092	0.96926	0.73839	1.08349	0.77007	1.71749
5	0.85776	1.02787	0.96187	0.71945	1.07970	0.73427	1.76205
6	0.85176	1.00231	0.95730	0.70558	1.07504	0.71181	1.77724
7	0.84582	0.98566	0.95275	0.69673	1.07161	0.69695	1.79178
8	0.84130	0.97467	0.94958	0.69067	1.06912	0.68675	1.80357
9	0.83802	0.96698	0.94715	0.68652	1.06697	0.67999	1.81054
10	0.83532	0.96185	0.94514	0.68378	1.06532	0.67543	1.81614
11	0.83323	0.95840	0.94361	0.68191	1.06403	0.67234	1.82032
12	0.83161	0.95604	0.94240	0.68065	1.06299	0.67025	1.82325

TABLE 34

EFFECT OF RECYCLE RATIO ON SEPARATION, TIME = 15.0 mins

NNZ	=	29
H	=	90.0 cm
Y_{Ao}	=	0.00095 gmoles/cc
Y_{Bo}	=	0.00086 gmoles/cc
Q	=	25.0 cc

TABLE 34

Beta = 0.00, TIME = 15 mins.

PHOT = PHOB = 0.70

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3		
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01575	1.91670
2	0.88749	0.90344	1.21962	0.70574	0.92420	1.32538	2.47828
3	0.79863	1.01264	1.18507	0.79469	0.79159	1.82762	3.44295
4	0.79622	1.01261	1.17157	0.83586	0.72494	2.02742	3.91991
5	0.79622	1.01261	1.17067	0.83586	0.71423	2.03462	3.98973
6	0.79622	1.01261	1.17065	0.83586	0.71332	2.03463	3.99477
7	0.79622	1.01261	1.17065	0.83586	0.71329	2.03463	3.99497
8	0.79622	1.01261	1.17065	0.83586	0.71329	2.03463	3.99497
9	0.79622	1.01261	1.17065	0.83586	0.71329	2.03463	3.99497
10	0.79622	1.01261	1.17065	0.83586	0.71329	2.03463	3.99497
11	0.79622	1.01261	1.17065	0.83586	0.71329	2.03463	3.99497
12	0.79622	1.01261	1.17065	0.83586	0.71329	2.03463	3.99497

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1		
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	1.24946	0.75028	0.96593	1.19178	0.97391	0.80460	2.05471
2	1.23311	0.77657	0.90158	1.43495	0.81669	0.98276	2.52729
3	1.21648	0.80287	0.82739	1.68368	0.61180	1.28839	3.08323
4	1.21620	0.80287	0.81709	1.68924	0.55784	1.41648	3.13170
5	1.21620	0.80287	0.81660	1.68924	0.55120	1.41711	3.13357
6	1.21620	0.80287	0.81659	1.68924	0.55084	1.41711	3.13361
7	1.21620	0.80287	0.81659	1.68924	0.55083	1.41711	3.13361
8	1.21620	0.80287	0.81659	1.68924	0.55083	1.41711	3.13361
9	1.21620	0.80287	0.81659	1.68924	0.55083	1.41711	3.13361
10	1.21620	0.80287	0.81659	1.68924	0.55083	1.41711	3.13361
11	1.21620	0.80287	0.81659	1.68924	0.55083	1.41711	3.13361
12	1.21620	0.80287	0.81659	1.68924	0.55083	1.41711	3.13361

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2		
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.98576	1.36739	0.78398	0.96694	1.23262	0.75939	2.25156
2	0.97708	1.36823	0.72464	1.08617	1.19674	0.79543	2.10680
3	0.96827	1.36907	0.66026	1.20548	1.14858	0.87726	1.85124
4	0.96814	1.36907	0.65507	1.20557	1.13479	0.92315	1.73833
5	0.96814	1.36907	0.65492	1.20557	1.13321	0.92326	1.73570
6	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559
7	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559
8	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559
9	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559
10	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559
11	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559
12	0.96814	1.36907	0.65492	1.20557	1.13314	0.92326	1.73559

TABLE 34 CONTINUED
 Beta = 0.20, TIME = 15 mins.
 PHOT = PHOB = 0.60

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01585	1.91689
2	0.89105	0.89051	1.23121	0.69034	0.91223	1.33603	2.61190
3	0.80313	0.98327	1.21010	0.75497	0.76460	1.86709	3.91443
4	0.80161	0.99566	1.19838	0.78720	0.70158	2.08112	4.51578
5	0.79437	1.00858	1.19600	0.79221	0.69507	2.10378	4.56941
6	0.79328	1.01077	1.19433	0.79778	0.69035	2.12691	4.61233
7	0.79271	1.01225	1.19399	0.79883	0.68879	2.13217	4.62677
8	0.79251	1.01268	1.19384	0.79949	0.68837	2.13487	4.63108
9	0.79245	1.01286	1.19379	0.79968	0.68820	2.13577	4.63290
10	0.79242	1.01293	1.19378	0.79977	0.68814	2.13613	4.63350
11	0.79242	1.01295	1.19377	0.79980	0.68812	2.13626	4.63372
12	0.79241	1.01296	1.19377	0.79981	0.68812	2.13631	4.63380

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.24946	0.75028	0.94862	1.21651	0.97877	0.80289	2.13563
2	1.23614	0.76773	0.88215	1.45839	0.82873	0.96210	2.66191
3	1.21916	0.78311	0.81629	1.70122	0.62923	1.23596	3.24454
4	1.21337	0.78858	0.81123	1.72113	0.58032	1.34909	3.26450
5	1.21112	0.79636	0.80404	1.74343	0.57683	1.35846	3.29764
6	1.21080	0.79735	0.80218	1.74871	0.57182	1.37071	3.31031
7	1.21058	0.79823	0.80166	1.75131	0.57062	1.37315	3.31309
8	1.21051	0.79844	0.80143	1.75220	0.57026	1.37454	3.31470
9	1.21049	0.79855	0.80136	1.75254	0.57010	1.37499	3.31515
10	1.21048	0.79858	0.80133	1.75268	0.57006	1.37517	3.31533
11	1.21048	0.79860	0.80132	1.75272	0.57004	1.37523	3.31539
12	1.21048	0.79860	0.80132	1.75274	0.57004	1.37526	3.31541

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.96741	1.37687	0.79574	0.94177	1.25186	0.72974	2.44159
2	0.97343	1.37325	0.73621	1.04926	1.21609	0.76166	2.25242
3	0.97081	1.38762	0.67852	1.15445	1.16916	0.83110	2.01075
4	0.96049	1.40983	0.67483	1.16330	1.15749	0.87005	1.95274
5	0.95843	1.41573	0.66840	1.17571	1.15570	0.87573	1.94936
6	0.95780	1.41811	0.66718	1.17806	1.15415	0.88064	1.94042
7	0.95750	1.41903	0.66672	1.17947	1.15378	0.88175	1.93923
8	0.95742	1.41936	0.66654	1.17991	1.15365	0.88234	1.93833
9	0.95739	1.41949	0.66648	1.18009	1.15360	0.88254	1.93806
10	0.95738	1.41954	0.66646	1.18015	1.15359	0.88261	1.93795
11	0.95738	1.41956	0.66646	1.18018	1.15358	0.88264	1.93791
12	0.95738	1.41956	0.66646	1.18019	1.15358	0.88265	1.93789

TABLE 34 CONTINUED

Beta = 0.40, TIME = 15 mins.
PHOT = PHOB = 0.50

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01593	1.91704
2	0.89572	0.88693	1.24272	0.67668	0.90105	1.34420	2.73984
3	0.81352	0.95426	1.23696	0.71662	0.73914	1.89793	4.43222
4	0.80669	0.96243	1.22641	0.73848	0.68224	2.11257	5.14240
5	0.79352	0.98615	1.21977	0.74989	0.67993	2.15200	5.14808
6	0.79135	0.99183	1.21613	0.76188	0.66945	2.20594	5.25986
7	0.78893	0.99838	1.21512	0.76586	0.66651	2.22139	5.28797
8	0.78806	1.00069	1.21433	0.76930	0.66505	2.23605	5.30717
9	0.78763	1.00253	1.21402	0.77071	0.66424	2.24193	5.31662
10	0.78741	1.00335	1.21386	0.77171	0.66392	2.24612	5.32150
11	0.78731	1.00399	1.21378	0.77219	0.66375	2.24814	5.32399
12	0.78726	1.00416	1.21374	0.77249	0.66367	2.24940	5.32535

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.24946	0.75028	0.93286	1.23845	0.98390	0.80112	2.21088
2	1.23915	0.75617	0.86401	1.47877	0.84609	0.93384	2.80470
3	1.21795	0.75744	0.80874	1.70659	0.65910	1.16570	3.39315
4	1.20168	0.76921	0.80858	1.74141	0.61624	1.25794	3.36453
5	1.19642	0.78530	0.79258	1.79317	0.61297	1.27361	3.44691
6	1.19545	0.78898	0.78912	1.80861	0.60205	1.29703	3.47270
7	1.19413	0.79338	0.78709	1.82256	0.59976	1.30312	3.48518
8	1.19377	0.79477	0.78598	1.82835	0.59823	1.30946	3.49402
9	1.19354	0.79600	0.78555	1.83236	0.59747	1.31186	3.49754
10	1.19343	0.79651	0.78531	1.83433	0.59718	1.31365	3.49978
11	1.19338	0.79687	0.78520	1.83554	0.59702	1.31449	3.50087
12	1.19336	0.79704	0.78515	1.83618	0.59695	1.31502	3.50148

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.95065	1.38483	0.80995	0.91084	1.27137	0.70053	2.64375
2	0.97314	1.36813	0.75226	1.00419	1.23642	0.72759	2.38906
3	0.97555	1.39582	0.70011	1.08875	1.19323	0.78183	2.18367
4	0.95321	1.44725	0.69327	1.10288	1.18377	0.81392	2.20820
5	0.94943	1.46355	0.68008	1.12635	1.17982	0.82772	2.19722
6	0.94682	1.47609	0.67787	1.13226	1.17653	0.83873	2.18689
7	0.94541	1.48185	0.67584	1.13863	1.17554	0.84326	2.18506
8	0.94488	1.48551	0.67499	1.14099	1.17491	0.84652	2.18205
9	0.94458	1.48742	0.67462	1.14278	1.17461	0.84805	2.18108
10	0.94444	1.48854	0.67442	1.14361	1.17448	0.84903	2.18026
11	0.94438	1.48915	0.67434	1.14414	1.17441	0.84953	2.17988
12	0.94434	1.48950	0.67429	1.14441	1.17437	0.84983	2.17964

TABLE 34 CONTINUED

Beta = 0.60, TIME = 15 mins.

PHOT = PHOB = 0.40

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01597	1.91712
2	0.89911	0.87847	1.25388	0.66698	0.89606	1.34345	2.81855
3	0.82748	0.92116	1.26482	0.68474	0.72732	1.90718	4.84361
4	0.81345	0.92457	1.25497	0.69666	0.67995	2.10621	5.57998
5	0.79649	0.95479	1.24198	0.71655	0.68216	2.15967	5.48741
6	0.79224	0.96475	1.23653	0.73585	0.66529	2.24410	5.66821
7	0.78661	0.98005	1.23386	0.74639	0.66144	2.27439	5.68431
8	0.78437	0.98672	1.23149	0.75651	0.65778	2.31517	5.72955
9	0.78266	0.99419	1.23036	0.76242	0.65567	2.33472	5.74631
10	0.78167	0.99825	1.22954	0.76773	0.65454	2.35467	5.76145
11	0.78106	1.00202	1.22904	0.77111	0.65378	2.36624	5.76873
12	0.78068	1.00436	1.22872	0.77389	0.65334	2.37638	5.77497

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.24946	0.75028	0.92493	1.25088	0.98931	0.79961	2.25221
2	1.24189	0.74346	0.85558	1.48858	0.86524	0.91088	2.90628
3	1.21423	0.72878	0.81524	1.68833	0.69604	1.10926	3.45044
4	1.18535	0.74659	0.82049	1.73471	0.66062	1.18116	3.35676
5	1.17719	0.76959	0.79558	1.81530	0.65472	1.20049	3.49021
6	1.17455	0.77806	0.79120	1.84512	0.63825	1.23145	3.52042
7	1.17079	0.78931	0.78598	1.88344	0.63455	1.24191	3.55445
8	1.16956	0.79416	0.78313	1.90246	0.63032	1.25705	3.57764
9	1.16843	0.79981	0.78158	1.92138	0.62825	1.26399	3.59134
10	1.16782	0.80279	0.78052	1.93259	0.62705	1.27140	3.61191
11	1.16744	0.80563	0.77991	1.94228	0.62626	1.27557	3.60882
12	1.16719	0.80737	0.77954	1.94864	0.62584	1.27932	3.61380

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.94202	1.38868	0.82218	0.88735	1.29143	0.67184	2.83363
2	0.98304	1.34875	0.76790	0.96968	1.25717	0.69924	2.46676
3	0.99106	1.38581	0.72063	1.03309	1.21969	0.74107	2.30138
4	0.95777	1.46446	0.70842	1.04898	1.21259	0.76805	2.41400
5	0.95320	1.49367	0.68973	1.07961	1.20491	0.79339	2.37979
6	0.94652	1.52715	0.68628	1.08970	1.19994	0.81262	2.38244
7	0.94301	1.54499	0.68098	1.10479	1.19754	0.82586	2.37573
8	0.94108	1.56167	0.67879	1.11153	1.19565	0.83639	2.37223
9	0.93975	1.57206	0.67730	1.11890	1.19459	0.84364	2.36875
10	0.93899	1.58072	0.67639	1.12298	1.19389	0.84931	2.36642
11	0.93852	1.58656	0.67587	1.12670	1.19343	0.85331	2.36431
12	0.93822	1.59114	0.67554	1.12905	1.19315	0.85636	2.36290

TABLE 34 CONTINUED
 Beta = 0.800, TIME = 15 mins.
 PHOT = PHOB = 0.30

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01602	1.91721
2	0.90551	0.86463	1.26568	0.65596	0.88637	1.34311	2.92377
3	0.84415	0.86965	1.29506	0.64223	0.71639	1.90401	5.35939
4	0.83548	0.85229	1.28549	0.63082	0.66848	2.05732	6.27158
5	0.81480	0.87426	1.26618	0.64554	0.66258	2.10130	6.22047
6	0.80331	0.88107	1.25760	0.66229	0.64445	2.18147	6.42767
7	0.79349	0.89843	1.25076	0.67538	0.63645	2.20672	6.42110
8	0.78728	0.90595	1.24577	0.68891	0.62982	2.26356	6.49907
9	0.78250	0.91830	1.24219	0.69928	0.62544	2.28984	6.50364
10	0.77918	0.92531	1.23958	0.71017	0.62232	2.32940	6.53344
11	0.77671	0.93422	1.23757	0.71884	0.62014	2.35307	6.53258
12	0.77493	0.94030	1.23613	0.72739	0.61855	2.38140	6.54262

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.24946	0.75028	0.91106	1.26803	0.99500	0.79778	2.31785
2	1.24589	0.72614	0.84223	1.50146	0.89205	0.87116	3.05877
3	1.21504	0.67991	0.79544	1.65458	0.75951	1.00874	3.71720
4	1.17825	0.68456	0.79563	1.69096	0.72232	1.04866	3.65806
5	1.16484	0.70246	0.76988	1.76855	0.70125	1.06076	3.80925
6	1.15606	0.71078	0.76005	1.79377	0.68166	1.08326	3.83857
7	1.14865	0.72391	0.75111	1.84737	0.67062	1.09026	3.90257
8	1.14409	0.73031	0.74531	1.87322	0.66200	1.10674	3.93735
9	1.14055	0.74032	0.74103	1.91105	0.65615	1.11417	3.97312
10	1.13807	0.74623	0.73807	1.93442	0.65210	1.12580	3.99713
11	1.13628	0.75365	0.73583	1.96198	0.64913	1.13261	4.02007
12	1.13494	0.75878	0.73428	1.98181	0.64712	1.14098	4.03699

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.92754	1.39450	0.84004	0.84868	1.31136	0.64367	3.06299
2	0.98840	1.31963	0.79346	0.91222	1.28052	0.66463	2.57229
3	1.00813	1.34948	0.74113	0.94288	1.24995	0.67509	2.47846
4	0.96575	1.42556	0.71836	0.94809	1.24179	0.68311	2.68334
5	0.95528	1.44988	0.69667	0.97079	1.22990	0.70754	2.63829
6	0.94229	1.49607	0.68581	0.97745	1.22288	0.72540	2.67655
7	0.93464	1.51975	0.67629	0.99431	1.21743	0.74427	2.65973
8	0.92888	1.55266	0.67030	1.00158	1.21355	0.75968	2.67021
9	0.92496	1.57396	0.66583	1.01348	1.21055	0.77442	2.65999
10	0.92198	1.59832	0.66271	1.02024	1.20842	0.78721	2.66112
11	0.91998	1.61636	0.66045	1.02879	1.20669	0.79896	2.65356
12	0.91840	1.63482	0.65882	1.03464	1.20544	0.80930	2.65141

TABLE 35

EFFECT OF RECYCLE RATIO, TIME = 30. mins.

NNZ	=	29
H	=	90.0 cm
Y_{Ao}	=	0.00095 gmole/cc
Y_{Bo}	=	0.00086 gmole/cc
Q	=	25.00 cm

TABLE 35

Beta = 0.00, TIME = 30 mins.

PHOT = PHOB = 0.70

CONCENTRATION TRANSIENTS IN STAGE 1

	T1	T2	T3	T1	T2	T3	
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.96896	0.78803	1.28562	0.64023	1.00000	1.01615	2.04046
2	0.96584	0.89369	1.27037	0.67934	0.89025	1.38931	2.97734
3	0.76131	1.00328	1.22629	0.80411	0.67173	1.02001	4.19390
4	0.76131	1.00328	1.22629	0.80411	0.67173	2.17511	4.80475
5	0.76131	1.00328	1.22629	0.80411	0.67193	2.13886	4.85439
6	0.76131	1.00328	1.22629	0.80411	0.67173	2.13886	4.85550
7	0.76131	1.00328	1.22629	0.80411	0.67178	2.13886	4.85551
8	0.76131	1.00328	1.22629	0.80411	0.67178	2.13886	4.85551
9	0.76131	1.00328	1.22629	0.80411	0.67178	2.13886	4.85551
10	0.76131	1.00328	1.22629	0.80411	0.67178	2.13886	4.85551
11	0.76131	1.00328	1.22629	0.80411	0.67173	2.13886	4.85551
12	0.76131	1.00328	1.22629	0.80411	0.67173	2.13886	4.85551

CONCENTRATION TRANSIENTS IN STAGE 2

	T2	T3	T1	T2	T3	T1	
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	1.29958	0.74840	0.90665	1.21798	0.96895	0.78808	2.33274
2	1.28651	0.77038	0.84237	1.48284	0.77359	0.98977	2.93968
3	1.27343	0.79237	0.77318	1.75064	0.51877	1.32714	3.63883
4	1.27341	0.79237	0.76823	1.75357	0.45680	1.46291	3.66839
5	1.27341	0.79237	0.76817	1.75357	0.45426	1.46300	3.66865
6	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865
7	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865
8	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865
9	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865
10	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865
11	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865
12	1.27341	0.79237	0.76817	1.75357	0.45423	1.46300	3.66865

CONCENTRATION TRANSIENTS IN STAGE 3

	T3	T1	T2	T3	T1	T2	
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.92863	1.41169	0.74705	0.97294	1.28364	0.75119	2.59771
2	0.92456	1.41136	0.66806	1.09724	1.24949	0.77073	2.47473
3	0.92050	1.41102	0.58737	1.22154	1.19915	0.83934	2.19002
4	0.92049	1.41102	0.58566	1.22153	1.18238	0.88841	2.04013
5	0.92049	1.41102	0.58565	1.22153	1.18180	0.88841	2.03911
6	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910
7	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910
8	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910
9	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910
10	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910
11	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910
12	0.92049	1.41102	0.58565	1.22153	1.18179	0.88841	2.03910

TABLE 35 CONTINUED

Beta = 0.20, TIME = 30 mins.

PHOT = PHOB = 0.60

CONCENTRATION TRANSIENTS IN STAGE 1

	T1	T2		T3			
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.96396	0.78803	1.28560	0.64023	1.00000	1.01630	2.04075
2	0.97115	0.89543	1.28397	0.66316	0.87934	1.37954	3.02868
3	0.77702	0.97047	1.27126	0.71751	0.70565	1.95619	4.91662
4	0.77267	0.92514	1.25930	0.74746	0.65755	2.13004	5.62237
5	0.76433	0.99683	1.25707	0.75106	0.65198	2.19950	5.64591
6	0.76417	0.99855	1.25532	0.75645	0.64869	2.22095	5.68182
7	0.76358	0.99976	1.25514	0.75721	0.64779	2.22493	5.69327
8	0.76342	1.00003	1.25501	0.75777	0.64760	2.22716	5.69572
9	0.76333	1.00021	1.25497	0.75791	0.64751	2.22783	5.69711
10	0.76336	1.00026	1.25496	0.75797	0.64748	2.22809	5.69745
11	0.76336	1.00027	1.25495	0.75799	0.64747	2.22818	5.69759
12	0.76336	1.00028	1.25495	0.75800	0.64747	2.22821	5.69763

CONCENTRATION TRANSIENTS IN STAGE 2

	T2	T3		T1			
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.29958	0.74840	0.88957	1.24529	0.97269	0.78709	2.43087
2	1.28992	0.76050	0.82412	1.50688	0.78566	0.96678	3.10137
3	1.27537	0.76919	0.76393	1.76662	0.53466	1.26670	3.83434
4	1.26775	0.77392	0.76446	1.78278	0.47603	1.38466	3.82013
5	1.26513	0.78207	0.75871	1.80323	0.47679	1.39300	3.84472
6	1.26502	0.78282	0.75757	1.80729	0.47159	1.40456	3.85514
7	1.26476	0.78365	0.75731	1.80939	0.47082	1.40645	3.85604
8	1.26472	0.78381	0.75716	1.81005	0.47056	1.40764	3.85730
9	1.26470	0.78390	0.75717	1.81030	0.47044	1.40798	3.85750
10	1.26469	0.78392	0.75712	1.81039	0.47042	1.40811	3.85761
11	1.26469	0.78393	0.75712	1.81042	0.47041	1.40816	3.85764
12	1.26469	0.78394	0.75712	1.81043	0.47041	1.40818	3.85765

CONCENTRATION TRANSIENTS IN STAGE 3

	T3	T1		T2			
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.91022	1.41794	0.60136	0.94561	1.30563	0.71808	2.83253
2	0.92082	1.41298	0.68189	1.05748	1.27395	0.72817	2.68459
3	0.92345	1.42540	0.60859	1.16664	1.22838	0.77621	2.44275
4	0.91400	1.44642	0.60842	1.17450	1.21514	0.81429	2.36154
5	0.91241	1.45142	0.60149	1.18597	1.21422	0.81849	2.35986
6	0.91207	1.45330	0.60068	1.18780	1.21255	0.82298	2.34767
7	0.91185	1.45402	0.60029	1.18898	1.21231	0.82377	2.34667
8	0.91181	1.45425	0.60014	1.18931	1.21220	0.82425	2.34557
9	0.91179	1.45434	0.60011	1.18944	1.21216	0.82438	2.34531
10	0.91178	1.45437	0.60010	1.18949	1.21215	0.82444	2.34520
11	0.91173	1.45438	0.60009	1.18950	1.21215	0.82446	2.34517
12	0.91173	1.45439	0.60009	1.18951	1.21214	0.82447	2.34515

TABLE 35 CONTINUED

Beta =0.40, TIME = 30 mins.

PHOT = PHOB = 0.5

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.96826	0.73626	1.25562	0.64023	1.00000	1.01634	2.24084
2	0.97708	0.87174	1.09737	0.65006	0.36891	1.37823	3.16552
3	0.77155	0.94007	1.20317	0.77217	0.60111	1.27060	5.50330
4	0.77215	0.94073	1.20245	0.77130	0.62442	2.19772	6.46979
5	0.77291	0.96899	1.20470	0.89892	0.63745	2.22923	6.42805
6	0.77155	0.97291	1.28120	0.70982	0.62929	2.23107	6.54261
7	0.76838	0.97879	1.28059	0.71239	0.62770	2.22223	6.56449
8	0.76323	0.93057	1.07970	0.71535	0.62604	2.37549	6.57989
9	0.76732	0.98207	1.27959	0.71629	0.62633	2.31012	6.58886
10	0.76763	0.98272	1.27943	0.71729	0.62618	2.31355	6.59222
11	0.76756	0.98312	1.27940	0.71742	0.62608	2.31515	6.59450
12	0.76752	0.98313	1.27937	0.71763	0.62604	2.31609	6.59547

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.29958	0.74840	0.87412	1.26826	0.97670	0.78598	2.51945
2	1.29304	0.74826	0.80691	1.52673	0.80341	0.93461	3.26964
3	1.27205	0.73862	0.75873	1.76455	0.56390	1.18636	4.00523
4	1.25040	0.74625	0.76544	1.79263	0.51089	1.27882	3.92415
5	1.24423	0.76173	0.75170	1.84283	0.51265	1.29152	4.00438
6	1.24382	0.76414	0.74962	1.85435	0.50084	1.31413	4.02657
7	1.24231	0.76821	0.74827	1.86678	0.49946	1.31840	4.03448
8	1.24207	0.76913	0.74748	1.87140	0.49799	1.32424	4.04311
9	1.24155	0.77018	0.74726	1.87463	0.49739	1.32613	4.04521
10	1.24176	0.77055	0.74710	1.87619	0.49718	1.32762	4.04700
11	1.24172	0.77033	0.74704	1.87709	0.49705	1.32829	4.04769
12	1.24170	0.77096	0.74701	1.87758	0.49700	1.32870	4.04816

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.89354	1.42291	0.77839	0.91146	1.32781	0.68596	3.08250
2	0.92151	1.40021	0.70070	1.00856	1.29942	0.68770	2.87107
3	0.92997	1.42401	0.63530	1.09335	1.26161	0.71419	2.70494
4	0.90814	1.47547	0.63316	1.10427	1.25186	0.73974	2.74951
5	0.90506	1.48856	0.61894	1.12658	1.24841	0.74916	2.74075
6	0.90328	1.49955	0.61756	1.13072	1.24513	0.75861	2.72478
7	0.90213	1.50426	0.61549	1.13653	1.24450	0.76160	2.72470
8	0.90182	1.50715	0.61481	1.13837	1.24388	0.76426	2.72200
9	0.90160	1.50863	0.61451	1.13986	1.24367	0.76529	2.71934
10	0.90152	1.50951	0.61434	1.14051	1.24356	0.76622	2.71824
11	0.90148	1.50998	0.61428	1.14091	1.24351	0.76636	2.71739
12	0.90146	1.51023	0.61425	1.14113	1.24348	0.76656	2.71761

TABLE 35 CONTINUED

Beta = 0.60, TIME = 30 mins.
PHOT = PHOB = 0.4

CONCENTRATION TRANSIENTS IN STAGE 1

T1 T2 T3

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.96826	0.78908	1.28560	0.64023	1.00000	1.01638	2.04091
2	0.70271	0.86475	1.70990	0.64164	0.86444	1.37315	3.24294
3	0.70271	0.70271	1.70271	0.4001	0.87047	1.01002	6.09984
4	0.70271	0.95151	1.70271	0.4517	0.63704	2.17522	7.03209
5	0.78741	0.92869	1.70287	0.65765	0.64242	2.21356	6.85740
6	0.78430	0.93412	1.30374	0.67323	0.62889	2.29391	7.06373
7	0.77829	0.94888	1.30184	0.67960	0.62709	2.31334	7.06656
8	0.77607	0.95380	1.29057	0.68799	0.62459	2.35396	7.11953
9	0.77493	0.96063	1.29877	0.69168	0.62325	2.36959	7.13898
10	0.77411	0.96400	1.29800	0.69610	0.62262	2.38793	7.15167
11	0.77356	0.96719	1.29767	0.69841	0.62213	2.39808	7.16190
12	0.77322	0.96905	1.29737	0.70059	0.62189	2.40684	7.16692

CONCENTRATION TRANSIENTS IN STAGE 2

T2 T3 T1

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.29958	0.74840	0.86586	1.28100	0.98100	0.78510	2.56905
2	1.29566	0.73505	0.79892	1.53642	0.82221	0.90894	3.38988
3	1.26486	0.70456	0.76812	1.73459	0.59958	1.12346	4.05407
4	1.22561	0.71404	0.78234	1.76975	0.55542	1.19017	3.88286
5	1.21604	0.73336	0.76051	1.84781	0.55630	1.20363	4.02885
6	1.21455	0.73781	0.75822	1.86749	0.53876	1.23204	4.05445
7	1.21041	0.74742	0.75426	1.90479	0.53672	1.23802	4.08973
8	1.20963	0.75007	0.75224	1.92000	0.53243	1.25309	4.11615
9	1.20843	0.75513	0.75124	1.93700	0.53086	1.25840	4.12623
10	1.20796	0.75715	0.75047	1.94676	0.52980	1.26522	4.13859
11	1.20762	0.75951	0.75008	1.95499	0.52915	1.26874	4.14409
12	1.20741	0.76081	0.74983	1.96072	0.52882	1.27196	4.14989

CONCENTRATION TRANSIENTS IN STAGE 3

T3 T1 T2

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.88445	1.42530	0.79227	0.88546	1.35021	0.65522	3.32080
2	0.93278	1.37034	0.71786	0.97142	1.32500	0.65650	2.96506
3	0.94825	1.40038	0.66075	1.02985	1.29698	0.66659	2.87343
4	0.91453	1.47853	0.65603	1.03942	1.29049	0.68085	3.06432
5	0.91099	1.49883	0.63668	1.06727	1.28269	0.69895	3.01937
6	0.90595	1.53078	0.63469	1.07303	1.27824	0.71371	3.02622
7	0.90306	1.54515	0.62926	1.08791	1.27649	0.72269	3.02218
8	0.90176	1.55981	0.62760	1.09307	1.27470	0.73122	3.01539
9	0.90069	1.56888	0.62620	1.09982	1.27393	0.73616	3.01430
10	0.90018	1.57612	0.62543	1.10327	1.27332	0.74074	3.00975
11	0.89983	1.58135	0.62498	1.10645	1.27297	0.74355	3.00864
12	0.89962	1.58512	0.62470	1.10855	1.27274	0.74592	3.00639

TABLE 35 CONTINUED

Beta = 0.80, TIME = 30 mins.

PHOT = PHOB = 0.30

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.94856	0.78808	1.28560	0.64024	1.00000	1.01642	2.04100
2	0.84119	0.84470	1.12240	0.53252	0.85516	1.37123	3.35359
3	0.77427	0.74245	1.07010	0.50274	0.63035	1.98966	6.29214
4	0.72124	0.62109	1.06100	0.37443	0.62002	2.10143	8.08254
5	0.68457	0.80702	1.03797	0.37870	0.63501	2.15325	7.83916
6	0.81706	0.83439	1.33185	0.58740	0.61876	2.22366	8.14836
7	0.80315	0.85196	1.32729	0.59314	0.61651	2.22379	8.07166
8	0.88430	0.85450	1.22311	0.80191	0.61171	2.20609	8.21646
9	0.83009	0.86613	1.02082	0.60616	0.60931	2.29908	8.22139
10	0.79773	0.87029	1.31862	0.51466	0.60738	2.33927	8.26234
11	0.70559	0.87800	1.31721	0.61914	0.60604	2.35726	8.27504
12	0.72416	0.88209	1.31607	0.62578	0.60504	2.38409	8.28668

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.29958	0.74840	0.85262	1.29805	0.98561	0.78383	2.64365
2	1.29938	0.71770	0.78422	1.55034	0.85008	0.86577	3.57916
3	1.26144	0.64902	0.76522	1.68710	0.65811	1.01768	4.28517
4	1.20776	0.63995	0.78623	1.71338	0.61877	1.04925	4.11282
5	1.19477	0.64976	0.76071	1.78178	0.61444	1.05543	4.30692
6	1.19027	0.65092	0.75781	1.78305	0.59454	1.07249	4.30251
7	1.18290	0.65956	0.75044	1.83868	0.58940	1.07129	4.39424
8	1.18027	0.66023	0.74690	1.85097	0.58126	1.08887	4.43017
9	1.17636	0.66896	0.74382	1.88706	0.57748	1.09174	4.46273
10	1.17511	0.67121	0.74182	1.90403	0.57403	1.10326	4.49361
11	1.17352	0.67730	0.74023	1.92852	0.57179	1.10763	4.51404
12	1.17246	0.68012	0.73911	1.94702	0.57012	1.11523	4.54118

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.87019	1.42898	0.81320	0.84261	1.37244	0.62601	3.60018
2	0.94229	1.32644	0.74582	0.91019	1.35267	0.62175	3.26253
3	0.96982	1.34870	0.69416	0.93109	1.33918	0.59714	3.11881
4	0.92896	1.41748	0.68597	0.92906	1.33610	0.58557	3.48158
5	0.92550	1.42067	0.66562	0.94552	1.32391	0.60158	3.38379
6	0.91557	1.46670	0.66081	0.94394	1.31927	0.60888	3.47398
7	0.91054	1.47790	0.65172	0.96136	1.31535	0.62048	3.44086
8	0.90664	1.50725	0.64820	0.96408	1.31225	0.63020	3.46310
9	0.90375	1.52311	0.64426	0.97566	1.31015	0.63888	3.45606
10	0.90170	1.54383	0.64199	0.97993	1.30840	0.64861	3.45380
11	0.89923	1.56008	0.64007	0.98755	1.30711	0.65599	3.45307
12	0.89906	1.57584	0.63876	0.99264	1.30606	0.66431	3.44602

TABLE 36

EFFECT OF CONCENTRATION ON SEPARATION, RECYCLE RATIO = 0.0
TIME = 10 mins

NNZ	=	29
H	=	90.0 cm
PHOT	=	0.70
PHOB	=	0.70
BETA	=	0.00
Q	=	25.0 cc

TABLE 36
 $Y_{Ao} = Y_{Bo} = 2.5\% \text{ V/V}$

CONCENTRATION TRANSIENTS IN STAGE 1

	T1	T2	T3				
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.93424	1.26541	2.10573	0.60950	1.00000	1.03511	3.57614
2	0.74887	1.30460	1.92124	0.68124	0.97960	0.95732	2.61261
3	0.54164	1.34863	1.49182	0.73820	0.80920	0.99420	2.33312
4	0.51943	1.35348	1.22266	0.72922	0.62650	1.09080	2.91929
5	0.51906	1.35349	1.17369	0.73510	0.57792	1.07710	2.97576
6	0.51906	1.35349	1.16877	0.73519	0.55838	1.08216	3.08096
7	0.51906	1.35349	1.16858	0.73519	0.55440	1.08284	3.10459
8	0.51906	1.35349	1.16858	0.73519	0.55404	1.08285	3.10660
9	0.51906	1.35349	1.16858	0.73519	0.55402	1.08285	3.10670
10	0.51906	1.35349	1.16858	0.73519	0.55402	1.08285	3.10671
11	0.51906	1.35349	1.16858	0.73519	0.55402	1.08285	3.10671
12	0.51906	1.35349	1.16858	0.73519	0.55402	1.08285	3.10671

CONCENTRATION TRANSIENTS IN STAGE 2

	T2	T3	T1				
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	2.13332	0.61204	0.98291	1.03946	0.93424	1.26692	3.68611
2	1.85325	0.64196	0.88977	1.03593	0.71272	1.37166	3.36109
3	1.56001	0.67236	0.73190	1.03012	0.43668	1.46378	3.26556
4	1.54667	0.67284	0.65251	1.03294	0.36583	1.45303	3.63891
5	1.54650	0.67284	0.63699	1.03811	0.34267	1.45748	3.74582
6	1.54650	0.67284	0.63611	1.03817	0.33449	1.46015	3.75119
7	1.54650	0.67284	0.63609	1.03817	0.33303	1.46025	3.75132
8	1.54650	0.67284	0.63609	1.03817	0.33292	1.46025	3.75132
9	1.54650	0.67284	0.63609	1.03817	0.33291	1.46025	3.75132
10	1.54650	0.67284	0.63609	1.03817	0.33291	1.46025	3.75132
11	1.54650	0.67284	0.63609	1.03817	0.33291	1.46025	3.75132
12	1.54650	0.67284	0.63609	1.03817	0.33291	1.46025	3.75132

CONCENTRATION TRANSIENTS IN STAGE 3

	T3	T1	T2				
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	1.01269	0.87700	0.55004	1.51077	2.12593	0.60576	3.03927
2	0.93346	0.90990	0.49970	1.44146	1.70588	0.70061	2.37340
3	0.85256	0.94302	0.42128	1.38595	1.20549	0.77805	1.71376
4	0.85088	0.94325	0.38819	1.40045	1.08890	0.76392	1.58017
5	0.85086	0.94325	0.38292	1.40114	1.04167	0.76803	1.50356
6	0.85086	0.94325	0.38267	1.40115	1.02913	0.76890	1.48376
7	0.85086	0.94325	0.38267	1.40115	1.02747	0.76892	1.48135
8	0.85086	0.94325	0.38267	1.40115	1.02736	0.76892	1.48119
9	0.85086	0.94325	0.38267	1.40115	1.02736	0.76892	1.48119
10	0.85086	0.94325	0.38267	1.40115	1.02736	0.76892	1.48118
11	0.85086	0.94325	0.38267	1.40115	1.02736	0.76892	1.48118
12	0.85086	0.94325	0.38267	1.40115	1.02736	0.76892	1.48118

TABLE 36 CONTINUED

$$Y_{Ao} = Y_{Bo} = 5\% \text{ V/V}$$

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.94755	0.96349	1.63577	0.60006	1.00000	1.02513	2.79455
2	0.76656	1.09055	1.53845	0.63839	0.90906	1.17816	3.12084
3	0.53306	1.21736	1.34141	0.72105	0.74064	1.49871	3.76450
4	0.57451	1.21811	1.23132	0.76500	0.63611	1.69598	4.29139
5	0.57447	1.21811	1.22061	0.76562	0.60337	1.72644	4.56169
6	0.57447	1.21811	1.22026	0.76563	0.59722	1.72715	4.60929
7	0.57447	1.21811	1.22025	0.76563	0.59673	1.72716	4.61302
8	0.57447	1.21811	1.22025	0.76563	0.59671	1.72716	4.61316
9	0.57447	1.21811	1.22025	0.76563	0.59671	1.72716	4.61317
10	0.57447	1.21811	1.22025	0.76563	0.59671	1.72716	4.61317
11	0.57447	1.21811	1.22025	0.76563	0.59671	1.72716	4.61317
12	0.57447	1.21811	1.22025	0.76563	0.59671	1.72716	4.61317

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.66150	0.60504	0.91113	1.12461	0.94754	0.96442	3.38953
2	1.56823	0.64428	0.84049	1.25429	0.68573	1.18830	3.63244
3	1.47351	0.68352	0.73467	1.40997	0.38692	1.53001	4.13728
4	1.47206	0.68353	0.69673	1.43614	0.33793	1.65619	4.43917
5	1.47205	0.68353	0.69390	1.43630	0.32409	1.66460	4.45777
6	1.47205	0.68353	0.69383	1.43630	0.32212	1.66467	4.45821
7	1.47205	0.68353	0.69383	1.43630	0.32199	1.66467	4.45821
8	1.47205	0.68353	0.69383	1.43630	0.32199	1.66467	4.45821
9	1.47205	0.68353	0.69383	1.43630	0.32199	1.66467	4.45821
10	1.47205	0.68353	0.69383	1.43630	0.32199	1.66467	4.45821
11	1.47205	0.68353	0.69383	1.43630	0.32199	1.66467	4.45821
12	1.47205	0.68353	0.69383	1.43630	0.32199	1.66467	4.45821

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.93795	1.16409	0.56923	1.20231	1.64563	0.60202	3.39256
2	0.91284	1.17923	0.49425	1.31876	1.43648	0.68281	2.71769
3	0.88748	1.19436	0.40687	1.43860	1.16471	0.80591	1.94494
4	0.88723	1.19435	0.39377	1.44199	1.08536	0.85033	1.71822
5	0.88723	1.19435	0.39307	1.44200	1.06687	0.85246	1.68474
6	0.88723	1.19435	0.39305	1.44200	1.06503	0.85247	1.68181
7	0.88723	1.19435	0.39305	1.44200	1.06494	0.85247	1.68166
8	0.88723	1.19435	0.39305	1.44200	1.06494	0.85247	1.68166
9	0.88723	1.19435	0.39305	1.44200	1.06494	0.85247	1.68166
10	0.88723	1.19435	0.39305	1.44200	1.06494	0.85247	1.68166
11	0.88723	1.19435	0.39305	1.44200	1.06494	0.85247	1.68166
12	0.88723	1.19435	0.39305	1.44200	1.06494	0.85247	1.68166

TABLE 36 CONTINUED
 $Y_{A0} = Y_{B0} = 10\% \text{ V/V}$

CONCENTRATION TRANSIENTS IN STAGE 1
 T1 T2 T3

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.97283	0.80793	1.26229	0.68414	1.00000	1.01451	1.87186
2	0.98135	0.90544	1.23422	0.73747	0.93251	1.29343	2.32134
3	0.78567	1.00294	1.19049	0.82912	0.80247	1.74868	3.13263
4	0.78178	1.00294	1.17315	0.86553	0.72624	1.93404	3.60925
5	0.78168	1.00294	1.17120	0.86561	0.71174	1.94311	3.69911
6	0.78168	1.00294	1.17112	0.86561	0.70877	1.94315	3.70919
7	0.78168	1.00294	1.17112	0.86561	0.70863	1.94315	3.70991
8	0.78168	1.00294	1.17112	0.86561	0.70862	1.94315	3.70995
9	0.78168	1.00294	1.17112	0.86561	0.70862	1.94315	3.70995
10	0.78168	1.00294	1.17112	0.86561	0.70862	1.94315	3.70995
11	0.78168	1.00294	1.17112	0.86561	0.70862	1.94315	3.70995
12	0.78168	1.00294	1.17112	0.86561	0.70862	1.94315	3.70995

CONCENTRATION TRANSIENTS IN STAGE 2
 T2 T3 T1

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.26959	0.77367	0.98269	1.17224	0.97283	0.80873	1.95753
2	1.24829	0.80042	0.91494	1.39744	0.81127	0.96326	2.38196
3	1.22631	0.82718	0.83359	1.62961	0.60221	1.23168	2.89821
4	1.22562	0.82719	0.81892	1.63660	0.54595	1.34693	2.96107
5	1.22560	0.82719	0.81781	1.63661	0.53635	1.34828	2.96508
6	1.22560	0.82719	0.81777	1.63661	0.53548	1.34828	2.96524
7	1.22560	0.82719	0.81777	1.63661	0.53543	1.34828	2.96525
8	1.22560	0.82719	0.81777	1.63661	0.53543	1.34828	2.96525
9	1.22560	0.82719	0.81777	1.63661	0.53543	1.34828	2.96525
10	1.22560	0.82719	0.81777	1.63661	0.53543	1.34828	2.96525
11	1.22560	0.82719	0.81777	1.63661	0.53543	1.34828	2.96525
12	1.22560	0.82719	0.81777	1.63661	0.53543	1.34828	2.96525

CONCENTRATION TRANSIENTS IN STAGE 3
 T3 T1 T2

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.00279	1.33400	0.77103	0.94581	1.25161	0.78771	2.11373
2	0.99079	1.33649	0.71168	1.05542	1.20726	0.82784	1.96716
3	0.97845	1.33898	0.64492	1.16546	1.14744	0.90782	1.72968
4	0.97811	1.33898	0.63712	1.16588	1.12916	0.94800	1.63057
5	0.97810	1.33898	0.63671	1.16588	1.12611	0.94832	1.62562
6	0.97810	1.33898	0.63670	1.16588	1.12586	0.94832	1.62526
7	0.97810	1.33898	0.63670	1.16588	1.12585	0.94832	1.62524
8	0.97810	1.33898	0.63670	1.16588	1.12585	0.94832	1.62524
9	0.97810	1.33898	0.63670	1.16588	1.12585	0.94832	1.62524
10	0.97810	1.33898	0.63670	1.16588	1.12585	0.94832	1.62524
11	0.97810	1.33898	0.63670	1.16588	1.12585	0.94832	1.62524
12	0.97810	1.33898	0.63670	1.16588	1.12585	0.94832	1.62524

TABLE 36 CONTINUED
 $Y_{A0} = Y_{B0} = 20\% V/V$

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.99494	0.75700	1.04810	0.80688	1.00000	1.00751	1.30870
2	0.98533	0.81716	1.04094	0.87565	1.01327	1.20497	1.41369
3	0.97247	0.87733	1.03105	0.96110	1.01568	1.45654	1.53844
4	0.96663	0.87733	1.02712	0.97793	0.99597	1.51222	1.59471
5	0.96446	0.87732	1.02546	0.97808	0.98337	1.51382	1.61400
6	0.96365	0.87731	1.02477	0.97808	0.97806	1.51385	1.62769
7	0.96335	0.87731	1.02448	0.97808	0.97588	1.51386	1.62487
8	0.96324	0.87731	1.02437	0.97808	0.97500	1.51386	1.62616
9	0.96320	0.87731	1.02432	0.97808	0.97464	1.51386	1.62667
10	0.96319	0.87731	1.02430	0.97808	0.97450	1.51386	1.62688
11	0.96318	0.87731	1.02429	0.97808	0.97444	1.51386	1.62696
12	0.96318	0.87731	1.02429	0.97808	0.97442	1.51386	1.62699

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.04557	0.96056	1.02989	1.12198	0.99494	0.75762	1.18583
2	1.04042	0.97480	1.02382	1.27487	0.97992	0.83326	1.32904
3	1.03333	0.98905	1.01072	1.43002	0.95809	0.97167	1.47819
4	1.03066	0.98908	1.00084	1.43229	0.94658	1.03579	1.49125
5	1.02966	0.98909	0.99687	1.43232	0.93983	1.03718	1.49576
6	1.02929	0.98909	0.99529	1.43232	0.93691	1.03721	1.49758
7	1.02915	0.98909	0.99467	1.43232	0.93569	1.03721	1.49831
8	1.02909	0.98909	0.99443	1.43232	0.93519	1.03721	1.49859
9	1.02907	0.98909	0.99434	1.43232	0.93498	1.03721	1.49870
10	1.02907	0.98909	0.99430	1.43232	0.93490	1.03721	1.49875
11	1.02906	0.98909	0.99429	1.43232	0.93486	1.03721	1.49876
12	1.02906	0.98909	0.99428	1.43232	0.93485	1.03721	1.49877

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2		
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.03246	1.26228	0.97021	0.79884	1.04421	0.97618	1.30781
2	1.02709	1.26328	0.96378	0.87621	1.03789	0.98873	1.29111
3	1.01967	1.26429	0.95289	0.95407	1.02808	1.02489	1.24376
4	1.01684	1.26430	0.94659	0.95455	1.02309	1.04944	1.21215
5	1.01577	1.26430	0.94402	0.95455	1.02095	1.05043	1.20978
6	1.01537	1.26430	0.94299	0.95455	1.02004	1.05042	1.20915
7	1.01522	1.26430	0.94259	0.95455	1.01965	1.05042	1.20887
8	1.01517	1.26430	0.94243	0.95455	1.01949	1.05042	1.20875
9	1.01514	1.26430	0.94236	0.95455	1.01943	1.05042	1.20870
10	1.01514	1.26430	0.94234	0.95455	1.01940	1.05042	1.20867
11	1.01513	1.26430	0.94233	0.95455	1.01939	1.05042	1.20866
12	1.01513	1.26430	0.94233	0.95455	1.01939	1.05042	1.20866

TABLE 37

EFFECT OF CONCENTRATION ON SEPARATION, RECYCLE RATIO = 0.00,
TIME = 14 mins.

NNZ	=	29
H	=	90.0 cm
PHOT	=	0.70
PHOB	=	0.70
BETA	=	0.00
Q	=	25.0 cc

TABLE 37

$$Y_{Ao} = Y_{Bo} = 2.5\% \text{ V/V}$$

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.93157	1.27377	2.14038	0.59884	1.00000	1.03576	3.70207
2	0.74492	1.31100	1.92964	0.67916	0.97773	0.95036	2.61856
3	0.54151	1.35153	1.37914	0.74196	0.80784	0.99798	2.27305
4	0.52451	1.35481	1.2161	0.72981	0.63279	1.08750	2.82962
5	0.52441	1.35481	1.16122	0.73521	0.58948	1.06880	2.86372
6	0.52441	1.35481	1.15855	0.73524	0.57075	1.07372	2.96434
7	0.52441	1.35481	1.15851	0.73524	0.56778	1.07404	2.98063
8	0.52441	1.35481	1.15851	0.73524	0.56765	1.07405	2.98136
9	0.52441	1.35481	1.15851	0.73524	0.56764	1.07405	2.98137
10	0.52441	1.35481	1.15851	0.73524	0.56764	1.07405	2.98137
11	0.52441	1.35481	1.15851	0.73524	0.56764	1.07405	2.98137
12	0.52441	1.35481	1.15851	0.73524	0.56764	1.07405	2.98137

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	2.16987	0.60092	0.96566	1.03424	0.93158	1.27495	3.86737
2	1.86216	0.63786	0.88536	1.03073	0.71415	1.37049	3.39872
3	1.54675	0.67498	0.73748	1.02963	0.44934	1.44289	3.19933
4	1.53901	0.67516	0.65779	1.03564	0.38798	1.42250	3.58886
5	1.53898	0.67516	0.64536	1.03925	0.36774	1.42707	3.67068
6	1.53898	0.67516	0.64503	1.03927	0.36051	1.42892	3.67261
7	1.53898	0.67516	0.64503	1.03927	0.35951	1.42895	3.67263
8	1.53898	0.67516	0.64503	1.03927	0.35947	1.42895	3.67263
9	1.53898	0.67516	0.64503	1.03927	0.35947	1.42895	3.67263
10	1.53898	0.67516	0.64503	1.03927	0.35947	1.42895	3.67263
11	1.53898	0.67516	0.64503	1.03927	0.35947	1.42895	3.67263
12	1.53898	0.67516	0.64503	1.03927	0.35947	1.42895	3.67263

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.99840	0.87056	0.54508	1.52549	2.16474	0.59425	3.17633
2	0.92625	0.90358	0.50472	1.43610	1.70463	0.70299	2.36549
3	0.85348	0.93664	0.43812	1.35996	1.17932	0.78508	1.64852
4	0.85286	0.93667	0.40812	1.37354	1.07951	0.76285	1.55416
5	0.85286	0.93667	0.40429	1.37388	1.03615	0.76779	1.48213
6	0.85286	0.93667	0.40421	1.37388	1.02660	0.76835	1.46741
7	0.85286	0.93667	0.40421	1.37388	1.02576	0.76835	1.46620
8	0.85286	0.93667	0.40421	1.37388	1.02573	0.76835	1.46616
9	0.85286	0.93667	0.40421	1.37388	1.02573	0.76835	1.46616
10	0.85286	0.93667	0.40421	1.37388	1.02573	0.76835	1.46616
11	0.85286	0.93667	0.40421	1.37388	1.02573	0.76835	1.46616
12	0.85286	0.93667	0.40421	1.37388	1.02573	0.76835	1.46616

TABLE 37 CONTINUED

$$Y_{Ao} = Y_{Bo} = 5\% \text{ V/V}$$

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.94461	0.96193	1.66604	0.58712	1.00000	1.02557	2.91026
2	0.75173	1.09702	1.56676	0.62587	0.90020	1.18303	3.28984
3	0.55576	1.23203	1.74724	0.71291	0.73291	1.51742	3.91257
4	0.55267	1.23195	1.21991	0.76133	0.64023	1.72098	4.30721
5	0.55267	1.23195	1.21271	0.76147	0.61093	1.74786	4.55640
6	0.55267	1.23195	1.21260	0.76147	0.60664	1.74812	4.58886
7	0.55267	1.23195	1.21260	0.76147	0.60645	1.74812	4.59031
8	0.55267	1.23195	1.21260	0.76147	0.60644	1.74812	4.59033
9	0.55267	1.23195	1.21260	0.76147	0.60644	1.74812	4.59033
10	0.55267	1.23195	1.21260	0.76147	0.60644	1.74812	4.59033
11	0.55267	1.23195	1.21260	0.76147	0.60644	1.74812	4.59033
12	0.55267	1.23195	1.21260	0.76147	0.60644	1.74812	4.59033

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.69537	0.59241	0.88204	1.12467	0.94459	0.96248	3.64903
2	1.59803	0.63305	0.82324	1.25428	0.67331	1.20374	3.84600
3	1.50006	0.67366	0.73149	1.40792	0.37332	1.57759	4.28586
4	1.49949	0.67365	0.69706	1.43197	0.33484	1.71579	4.57272
5	1.49949	0.67365	0.69557	1.43198	0.32400	1.72140	4.58252
6	1.49949	0.67365	0.69556	1.43198	0.32287	1.72141	4.58262
7	1.49949	0.67365	0.69556	1.43198	0.32283	1.72141	4.58262
8	1.49949	0.67365	0.69556	1.43198	0.32283	1.72141	4.58262
9	1.49949	0.67365	0.69556	1.43198	0.32283	1.72141	4.58262
10	1.49949	0.67365	0.69556	1.43198	0.32283	1.72141	4.58262
11	1.49949	0.67365	0.69556	1.43198	0.32283	1.72141	4.58262
12	1.49949	0.67365	0.69556	1.43198	0.32283	1.72141	4.58262

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.90996	1.16892	0.54410	1.21788	1.68207	0.58687	3.68183
2	0.89127	1.17863	0.47277	1.34402	1.44542	0.67178	2.84534
3	0.87253	1.18833	0.39233	1.47165	1.14259	0.80515	1.93272
4	0.87247	1.18833	0.38294	1.47314	1.06217	0.85488	1.69229
5	0.87247	1.18833	0.38265	1.47314	1.04703	0.85613	1.66574
6	0.87247	1.18833	0.38265	1.47314	1.04612	0.85613	1.66429
7	0.87247	1.18833	0.38265	1.47314	1.04610	0.85613	1.66426
8	0.87247	1.18833	0.38265	1.47314	1.04610	0.85613	1.66426
9	0.87247	1.18833	0.38265	1.47314	1.04610	0.85613	1.66426
10	0.87247	1.18833	0.38265	1.47314	1.04610	0.85613	1.66426
11	0.87247	1.18833	0.38265	1.47314	1.04610	0.85613	1.66426
12	0.87247	1.18833	0.38265	1.47314	1.04610	0.85613	1.66426

TABLE 37 CONTINUED
 $Y_{A0} = Y_{B0} = 10\% \text{ V/V}$

CONCENTRATION TRANSIENTS IN STAGE 1
 T1 T2 T3

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.96978	0.79506	1.28837	0.67161	1.00000	1.01481	1.94675
2	0.86795	0.89423	1.26262	0.72306	0.91279	1.31835	2.52209
3	0.76377	0.99337	1.21074	0.81331	0.76787	1.80524	3.52293
4	0.76140	0.99374	1.19944	0.85211	0.69886	1.99510	4.01849
5	0.76138	0.99334	1.19827	0.85211	0.68652	2.00163	4.10007
6	0.76138	0.99334	1.19825	0.85211	0.68543	2.00165	4.10651
7	0.76138	0.99334	1.19825	0.85211	0.68539	2.00165	4.10676
8	0.76138	0.99334	1.19825	0.85211	0.68539	2.00165	4.10676
9	0.76138	0.99334	1.19825	0.85211	0.68539	2.00165	4.10676
10	0.76138	0.99334	1.19825	0.85211	0.68539	2.00165	4.10676
11	0.76138	0.99334	1.19825	0.85211	0.68539	2.00165	4.10676
12	0.76138	0.99334	1.19825	0.85211	0.68539	2.00165	4.10676

CONCENTRATION TRANSIENTS IN STAGE 2
 T2 T3 T1

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	1.29865	0.77411	0.95015	1.18915	0.96978	0.79549	2.09957
2	1.27838	0.79928	0.88133	1.42652	0.78585	0.96156	2.58882
3	1.25784	0.82445	0.80135	1.66887	0.55033	1.24865	3.17733
4	1.25757	0.82445	0.78969	1.67384	0.49198	1.37029	3.23319
5	1.25757	0.82445	0.78917	1.67384	0.48485	1.37090	3.23531
6	1.25757	0.82445	0.78916	1.67384	0.48446	1.37090	3.23534
7	1.25757	0.82445	0.78916	1.67384	0.48445	1.37090	3.23534
8	1.25757	0.82445	0.78916	1.67384	0.48445	1.37090	3.23534
9	1.25757	0.82445	0.78916	1.67384	0.48445	1.37090	3.23534
10	1.25757	0.82445	0.78916	1.67384	0.48445	1.37090	3.23534
11	1.25757	0.82445	0.78916	1.67384	0.48445	1.37090	3.23534
12	1.25757	0.82445	0.78916	1.67384	0.48445	1.37090	3.23534

CONCENTRATION TRANSIENTS IN STAGE 3
 T3 T1 T2

M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	SFACTOR
1	0.97233	1.36260	0.74787	0.94439	1.28058	0.78505	2.28595
2	0.96289	1.36345	0.67823	1.05792	1.23431	0.81685	2.13964
3	0.95335	1.36430	0.60321	1.17154	1.16981	0.89132	1.87819
4	0.95324	1.36430	0.59769	1.17164	1.14933	0.93408	1.76101
5	0.95324	1.36430	0.59755	1.17164	1.14698	0.93419	1.75721
6	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706
7	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706
8	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706
9	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706
10	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706
11	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706
12	0.95324	1.36430	0.59755	1.17164	1.14688	0.93419	1.75706

TABLE 37 CONTINUED
 $Y_{A0} = Y_{B0} = 20\% \text{ V/V}$

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.99366	0.73457	1.05853	0.79935	1.00000	1.00776	1.33450
2	0.98014	0.79413	1.04942	0.87123	1.01068	1.22007	1.45408
3	0.96187	0.85367	1.03749	0.95871	1.00613	1.47612	1.58769
4	0.95577	0.85364	1.03366	0.97438	0.98147	1.52069	1.64366
5	0.95404	0.85364	1.03231	0.97444	0.96881	1.52151	1.66379
6	0.95356	0.85363	1.03185	0.97444	0.96450	1.52153	1.67046
7	0.95342	0.85363	1.03170	0.97444	0.96311	1.52153	1.67264
8	0.95338	0.85363	1.03165	0.97444	0.96266	1.52153	1.67334
9	0.95337	0.85363	1.03164	0.97444	0.96252	1.52153	1.67355
10	0.95337	0.85363	1.03163	0.97444	0.96248	1.52153	1.67362
11	0.95337	0.85363	1.03163	0.97444	0.96247	1.52153	1.67364
12	0.95337	0.85363	1.03163	0.97444	0.96246	1.52153	1.67365

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.05571	0.97768	1.03077	1.13626	0.99366	0.73487	1.19033
2	1.04937	0.99051	1.02117	1.29370	0.97116	0.81622	1.34216
3	1.04119	1.00335	1.00390	1.45249	0.93981	0.96517	1.50140
4	1.03882	1.00337	0.99376	1.45385	0.92587	1.03348	1.51466
5	1.03814	1.00338	0.99053	1.45386	0.91901	1.03441	1.51861
6	1.03795	1.00338	0.98953	1.45386	0.91660	1.03442	1.51986
7	1.03790	1.00338	0.98923	1.45386	0.91580	1.03442	1.52024
8	1.03788	1.00338	0.98914	1.45386	0.91554	1.03442	1.52036
9	1.03788	1.00338	0.98911	1.45386	0.91546	1.03442	1.52040
10	1.03788	1.00338	0.98910	1.45386	0.91544	1.03442	1.52041
11	1.03788	1.00338	0.98910	1.45386	0.91543	1.03442	1.52041
12	1.03788	1.00338	0.98910	1.45386	0.91543	1.03442	1.52041

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.03474	1.28224	0.95824	0.78282	1.05295	0.99159	1.31587
2	1.02842	1.28256	0.94958	0.86204	1.04472	0.99305	1.31200
3	1.02025	1.28288	0.93618	0.94148	1.03284	1.01869	1.27489
4	1.01786	1.28289	0.92968	0.94170	1.02791	1.04341	1.24165
5	1.01718	1.28289	0.92761	0.94170	1.02615	1.04395	1.23972
6	1.01698	1.28289	0.92696	0.94170	1.02555	1.04396	1.23922
7	1.01693	1.28289	0.92677	0.94170	1.02534	1.04396	1.23904
8	1.01692	1.28289	0.92671	0.94170	1.02528	1.04396	1.23897
9	1.01691	1.28289	0.92669	0.94170	1.02526	1.04396	1.23895
10	1.01691	1.28289	0.92668	0.94170	1.02525	1.04396	1.23895
11	1.01691	1.28289	0.92668	0.94170	1.02525	1.04396	1.23895
12	1.01691	1.28289	0.92668	0.94170	1.02525	1.04396	1.23894

TABLE 38

EFFECT OF CONCENTRATION ON SEPARATION, RECYCLE RATIO = 1.00,
TIME = 10 mins.

NNZ	=	29
H	=	90.0 cm
PHOT	=	0.20
PHOB	=	0.20
BETA	=	1.00
Q	=	25.0 cc

TABLE 38
 $Y_{Ao} = Y_{Bo} = 2.5\% \text{ V/V}$

CONCENTRATION TRANSIENTS IN STAGE 1

	T1	T2	T3				
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.93424	1.26541	2.10573	0.60950	1.01000	1.03575	3.57837
2	0.73287	1.33449	2.06406	0.64467	1.00812	0.97995	3.11195
3	0.70898	1.35887	1.89084	0.69028	0.94637	0.94571	2.73733
4	0.80425	1.38618	1.84228	0.70557	0.86315	0.91969	2.78208
5	0.70416	1.43362	1.81736	0.73874	0.85933	0.95070	2.72165
6	0.69558	1.41442	1.68778	0.75396	0.83765	1.04640	2.79640
7	0.68173	1.45369	1.66517	0.74858	0.79922	1.02130	2.84254
8	0.64946	1.47629	1.62932	0.76910	0.78846	1.04647	2.81173
9	0.63751	1.47162	1.57867	0.77613	0.77396	1.11883	2.94037
10	0.62624	1.49455	1.55465	0.77632	0.75739	1.10432	2.91991
11	0.61234	1.50664	1.53217	0.78825	0.74777	1.12957	2.93622
12	0.60348	1.50773	1.50805	0.79217	0.73889	1.17611	3.03115

CONCENTRATION TRANSIENTS IN STAGE 2

	T2	T3	T1				
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	2.13332	0.61204	0.86803	1.14958	0.94871	1.25834	4.61611
2	1.91741	0.63921	0.90219	1.02592	0.71755	1.47561	3.41102
3	1.72219	0.74136	0.95318	0.87184	0.46839	1.63303	2.12478
4	1.67099	0.82152	0.94932	0.93598	0.45522	1.47887	2.00542
5	1.59250	0.79917	0.88938	1.03244	0.45560	1.53763	2.31323
6	1.58508	0.81120	0.84936	0.99690	0.43865	1.67205	2.29344
7	1.55379	0.85287	0.84030	1.02053	0.42446	1.61038	2.21259
8	1.51437	0.84300	0.81680	1.08078	0.42012	1.65293	2.37700
9	1.49957	0.85371	0.79637	1.06373	0.41269	1.72872	2.34624
10	1.48136	0.87711	0.78582	1.08398	0.40572	1.70424	2.32972
11	1.46198	0.87388	0.77383	1.11944	0.40170	1.73367	2.42020
12	1.44980	0.88211	0.76300	1.11376	0.39764	1.77317	2.39909

CONCENTRATION TRANSIENTS IN STAGE 3

	T3	T1	T2				
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.89208	0.94137	0.52794	1.55472	2.53007	0.56371	4.73629
2	1.09700	0.92374	0.49885	1.53986	2.16156	0.65615	2.77400
3	1.15446	1.08121	0.52004	1.45130	1.73297	0.74099	2.19033
4	0.96952	1.23103	0.53694	1.49707	1.71656	0.71309	3.05649
5	0.94468	1.15039	0.48806	1.59339	1.69345	0.73533	2.80445
6	0.93118	1.18942	0.47492	1.54882	1.59857	0.76949	2.65359
7	0.88746	1.27296	0.46911	1.58754	1.56584	0.75553	2.97278
8	0.86525	1.23879	0.45422	1.63672	1.53927	0.77065	2.85967
9	0.85102	1.26750	0.44533	1.62061	1.50195	0.78748	2.84069
10	0.83267	1.31379	0.43972	1.64543	1.47841	0.78308	2.97880
11	0.81887	1.30109	0.43298	1.67071	1.46033	0.79257	2.92758
12	0.80900	1.32081	0.42771	1.66683	1.44180	0.80100	2.93877

TABLE 38 CONTINUED

$$Y_{A0} = Y_{B0} = 5\% \text{ V/V}$$

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.94755	0.96349	1.63577	0.60006	0.99999	1.02554	2.79567
2	0.78315	1.03874	1.69947	0.56757	0.88757	1.25135	4.22147
3	0.67741	1.02200	1.73239	0.54367	0.73617	1.66595	7.21096
4	0.68867	0.95541	1.66233	0.53909	0.70880	1.56851	6.82247
5	0.63699	0.95660	1.57109	0.53991	0.70378	1.34026	5.54161
6	0.61688	0.93148	1.51188	0.53725	0.67075	1.38391	5.80616
7	0.58673	0.93062	1.47259	0.52304	0.65022	1.32524	5.73825
8	0.56592	0.92434	1.42225	0.52371	0.63514	1.29598	5.54130
9	0.55016	0.91855	1.38870	0.51923	0.61789	1.29183	5.59177
10	0.53462	0.91718	1.35826	0.51692	0.60624	1.26905	5.50042
11	0.52339	0.91417	1.33152	0.51605	0.59561	1.26406	5.47602
12	0.51372	0.91279	1.31090	0.51439	0.58659	1.25718	5.46188

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	1.66150	0.60504	0.81092	1.26965	0.97514	0.95380	4.29952
2	1.62162	0.60734	0.78372	1.38588	0.72738	1.08382	4.72152
3	1.46695	0.61955	0.81485	1.25343	0.44389	1.27584	3.64218
4	1.30767	0.65632	0.82862	1.06111	0.41701	1.24950	2.55148
5	1.26243	0.64654	0.76708	1.11459	0.40343	1.18686	2.83718
6	1.22916	0.61943	0.74458	1.06657	0.37357	1.20028	2.84245
7	1.18348	0.62344	0.72133	1.03684	0.35966	1.17825	2.72866
8	1.15751	0.61364	0.69654	1.03600	0.34568	1.17251	2.80558
9	1.13168	0.61062	0.68103	1.01609	0.33408	1.16983	2.76512
10	1.11039	0.60907	0.66517	1.01198	0.32593	1.16280	2.77362
11	1.09430	0.60595	0.65265	1.00664	0.31855	1.16154	2.78544
12	1.08007	0.60518	0.64264	1.00136	0.31285	1.15902	2.78093

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0	
1	0.83181	1.30275	0.62215	1.09309	1.88941	0.51534	5.74208
2	1.01779	1.11636	0.54093	1.16362	1.77359	0.53010	3.66974
3	1.09775	0.99953	0.49482	1.14214	1.62358	0.55162	2.67994
4	0.97550	1.07955	0.49366	1.07759	1.57625	0.53903	3.23610
5	0.94803	1.04309	0.45084	1.08785	1.51160	0.52872	3.14564
6	0.90553	1.01266	0.43525	1.06383	1.44807	0.52894	3.06161
7	0.86551	1.01579	0.41488	1.05977	1.41031	0.51958	3.18564
8	0.84115	0.99845	0.39875	1.05578	1.36518	0.51875	3.12382
9	0.81384	0.99518	0.38759	1.04903	1.33253	0.51630	3.15592
10	0.79392	0.99137	0.37659	1.04773	1.30508	0.51419	3.16937
11	0.77740	0.98668	0.36845	1.04499	1.28066	0.51355	3.16508
12	0.76297	0.98543	0.36172	1.04334	1.26174	0.51243	3.18020

TABLE 38 CONTINUED
 $Y_{Ao} = Y_{Bo} = 10\% V/V$

CONCENTRATION TRANSIENTS IN STAGE 1							
	T1		T2		T3		
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.97283	0.80793	1.26229	0.68414	1.00000	1.01468	1.87218
2	0.90446	0.85118	1.29851	0.68172	0.89599	1.27345	2.73717
3	0.85521	0.81500	1.35249	0.64276	0.74700	1.68849	4.75624
4	0.86601	0.75720	1.35152	0.59681	0.70761	1.74177	5.57418
5	0.85015	0.75605	1.33253	0.58051	0.70271	1.71201	5.59239
6	0.83702	0.74383	1.32530	0.56938	0.68700	1.71877	5.82332
7	0.82597	0.74135	1.31633	0.56192	0.67649	1.68390	5.83101
8	0.81651	0.73255	1.31010	0.55436	0.66723	1.67802	5.94345
9	0.80871	0.72909	1.30410	0.54758	0.65970	1.65216	5.96437
10	0.80203	0.72236	1.29958	0.54128	0.65339	1.64228	6.03465
11	0.79651	0.71856	1.29542	0.53529	0.64818	1.62257	6.05793
12	0.79182	0.71320	1.29220	0.52996	0.64380	1.61125	6.10231

CONCENTRATION TRANSIENTS IN STAGE 2							
	T2		T3		T1		
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	1.26959	0.77367	0.90985	1.24657	1.00357	0.79701	2.24830
2	1.26930	0.73068	0.84800	1.43670	0.92137	0.81458	2.94311
3	1.23958	0.64425	0.81338	1.51787	0.83387	0.85781	3.59054
4	1.20745	0.60890	0.82310	1.48951	0.81190	0.85841	3.58849
5	1.19624	0.60238	0.80180	1.49823	0.78944	0.84843	3.71069
6	1.18433	0.59335	0.79079	1.46031	0.77334	0.84853	3.68596
7	1.17558	0.58982	0.77968	1.45423	0.75819	0.84129	3.71747
8	1.16748	0.58281	0.77121	1.42656	0.74652	0.83816	3.70548
9	1.16115	0.57898	0.76374	1.41624	0.73590	0.83183	3.71898
10	1.15547	0.57328	0.75777	1.39541	0.72751	0.82904	3.71157
11	1.15095	0.56957	0.75260	1.38358	0.72002	0.82410	3.71493
12	1.14696	0.56492	0.74842	1.36709	0.71401	0.82113	3.70860

CONCENTRATION TRANSIENTS IN STAGE 3							
	T3		T1		T2		
M	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	SFACTOR
1	0.92725	1.36192	0.84657	0.79839	1.36199	0.64827	3.08583
2	1.01605	1.26618	0.81133	0.83185	1.32955	0.67605	2.45079
3	1.06078	1.25803	0.76835	0.82452	1.30430	0.66190	2.33695
4	1.02042	1.27406	0.75103	0.80438	1.30212	0.62978	2.58149
5	1.01226	1.23627	0.73358	0.80538	1.29170	0.62155	2.53808
6	0.99723	1.23081	0.71969	0.79531	1.28565	0.60622	2.61749
7	0.98743	1.20368	0.70831	0.79358	1.27920	0.59925	2.60217
8	0.97792	1.19388	0.69841	0.78609	1.27462	0.58831	2.64501
9	0.97076	1.17376	0.69038	0.78331	1.27022	0.58117	2.64266
10	0.96422	1.16250	0.68343	0.77760	1.26695	0.57261	2.66760
11	0.95913	1.14677	0.67774	0.77444	1.26394	0.56591	2.67041
12	0.95460	1.13555	0.67286	0.76990	1.26164	0.55895	2.68501

TABLE 38 CONTINUED
 $Y_{Ao} = Y_{Bo} = 20\% \text{ V/V}$

CONCENTRATION TRANSIENTS IN STAGE 1

M	T1		T2		T3		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	0.99494	0.75700	1.04810	0.80688	1.00000	1.00765	1.30888
2	0.98664	0.77847	1.05555	0.86924	0.99612	1.16074	1.41501
3	0.97398	0.72691	1.06824	0.90907	0.98207	1.38733	1.65993
4	0.97721	0.67179	1.06762	0.88327	0.96624	1.44027	1.80171
5	0.97041	0.68486	1.05924	0.88030	0.95964	1.45209	1.82075
6	0.96327	0.69299	1.05508	0.89408	0.95310	1.47621	1.82777
7	0.95813	0.70596	1.05099	0.91275	0.94478	1.48384	1.80844
8	0.95377	0.71813	1.04679	0.93261	0.93986	1.49774	1.78866
9	0.95018	0.73352	1.04386	0.95566	0.93556	1.50506	1.75720
10	0.94744	0.75081	1.04133	0.98252	0.93175	1.51507	1.72338
11	0.94527	0.77284	1.03905	1.01469	0.92901	1.52127	1.67683
12	0.94359	0.79749	1.03726	1.05419	0.92688	1.52820	1.62226

CONCENTRATION TRANSIENTS IN STAGE 2

M	T2		T3		T1		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.04557	0.96056	1.01180	1.14944	1.00546	0.74825	1.23658
2	1.04620	0.90294	0.99840	1.27600	1.00433	0.71417	1.48083
3	1.04352	0.78555	0.98439	1.38198	1.00562	0.69903	1.86493
4	1.03990	0.73565	0.98044	1.40213	1.00020	0.70388	2.02156
5	1.03544	0.74326	0.97284	1.43194	0.98938	0.71175	2.05052
6	1.02875	0.75408	0.96569	1.44179	0.98435	0.72943	2.03684
7	1.02457	0.77086	0.96019	1.45942	0.97948	0.74376	2.02018
8	1.02105	0.78731	0.95553	1.47016	0.97470	0.76319	1.99534
9	1.01773	0.80774	0.95181	1.48485	0.97149	0.78243	1.96559
10	1.01522	0.83026	0.94888	1.49561	0.96880	0.80730	1.92730
11	1.01312	0.85955	0.94658	1.50818	0.96650	0.83104	1.87796
12	1.01132	0.89214	0.94480	1.51701	0.96488	0.85999	1.82013

CONCENTRATION TRANSIENTS IN STAGE 3

M	T3		T1		T2		SFACTOR
	YA1/YAO	YB1/YBO	YA2/YAO	YB2/YBO	YA3/YAO	YB3/YBO	
1	1.01508	1.25081	0.98043	0.67276	1.07160	0.88509	1.49188
2	1.02880	1.25406	0.97679	0.68472	1.05895	0.93494	1.38065
3	1.03214	1.31396	0.96880	0.66805	1.04394	0.96965	1.37058
4	1.01760	1.35451	0.96417	0.65956	1.03892	0.97448	1.41909
5	1.01171	1.36734	0.95872	0.67360	1.03349	0.99169	1.40849
6	1.00562	1.39075	0.95096	0.68284	1.02856	1.00897	1.40983
7	0.99876	1.40526	0.94634	0.69687	1.02484	1.03207	1.39716
8	0.99448	1.42569	0.94233	0.71058	1.02174	1.05522	1.38811
9	0.99073	1.44198	0.93871	0.72841	1.01910	1.08350	1.36896
10	0.98739	1.46185	0.93611	0.74840	1.01700	1.11527	1.35007
11	0.98494	1.47822	0.93408	0.77386	1.01525	1.15263	1.32193
12	0.98294	1.49551	0.93242	0.79880	1.01383	1.19065	1.29553

NN7= 29 H= 90.00000 TIME= 15.00000
 PHOT= 0.36500 PHOB= 0.03500 BETA= 1.00000
 YBO= 0.00095 YCO= 0.00086

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01565
2	0.91970	0.83462	1.28011	0.63940	0.89618	1.24747
3	0.89300	0.76439	1.34044	0.57529	0.75872	1.58507
4	0.92427	0.67093	1.35184	0.48258	0.73619	1.54154
5	0.92705	0.64533	1.74707	0.42692	0.74623	1.39797
6	0.92870	0.60008	1.75174	0.39890	0.74473	1.32315
7	0.93193	0.58063	1.35312	0.37659	0.74555	1.20930
8	0.93440	0.56634	1.35598	0.36565	0.74742	1.14587
9	0.93730	0.55577	1.35782	0.35479	0.74933	1.09072
10	0.93958	0.54772	1.35984	0.34907	0.75161	1.05543
11	0.94176	0.54221	1.36141	0.34416	0.75369	1.03333
12	0.94356	0.53833	1.36283	0.34123	0.75567	1.01647

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.24946	0.75028	0.89026	1.27689	1.00098	0.79475
2	1.25305	0.70263	0.83921	1.44030	0.94409	0.77416
3	1.23857	0.57386	0.82254	1.43683	0.89246	0.76209
4	1.22503	0.49091	0.85103	1.28799	0.89002	0.73691
5	1.22689	0.46257	0.84753	1.20810	0.88748	0.70477
6	1.22703	0.43520	0.85024	1.07078	0.89048	0.69151
7	1.22959	0.42303	0.85215	0.99681	0.89122	0.67100
8	1.23098	0.40867	0.85488	0.93284	0.89452	0.66012
9	1.23323	0.40117	0.85735	0.89226	0.89671	0.64902
10	1.23489	0.39412	0.85976	0.86753	0.89955	0.64255
11	1.23664	0.38999	0.86187	0.84835	0.90182	0.63793
12	1.23805	0.38705	0.86375	0.83756	0.90400	0.63466

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.90795	1.39014	0.87379	0.76337	1.33503	0.60876
2	0.99304	1.24068	0.84905	0.78169	1.31700	0.59452
3	1.05012	1.12964	0.82455	0.74280	1.31218	0.52833
4	1.03310	1.06113	0.82707	0.69156	1.32291	0.44607
5	1.04081	0.91456	0.82747	0.67398	1.32379	0.40383
6	1.04084	0.84333	0.82821	0.64540	1.32775	0.37692
7	1.04466	0.78468	0.83096	0.63067	1.32992	0.35842
8	1.04708	0.74851	0.83290	0.61550	1.33243	0.34870
9	1.05017	0.72772	0.83558	0.60681	1.33429	0.34020
10	1.05259	0.71130	0.83769	0.60058	1.33594	0.33566
11	1.05485	0.70233	0.83983	0.59622	1.33729	0.33204
12	1.05677	0.69548	0.84161	0.59359	1.33841	0.32984

NN7= 29 H= 70.0000 TIME= 15.0000
 PHOT= 0.10000 PHOB= 0.30000 BETA= 1.00000
 YBO= 0.00095 YCO= 0.00086

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97391	0.80421	1.24155	0.65796	1.00000	1.01602
2	0.90568	0.86415	1.27662	0.65091	0.89100	1.33013
3	0.85685	0.84706	1.32814	0.61144	0.72799	1.88528
4	0.86416	0.81966	1.32236	0.58462	0.69066	1.97789
5	0.84503	0.82429	1.39929	0.60096	0.69111	2.01425
6	0.83041	0.83193	1.39024	0.61195	0.67180	2.06587
7	0.81707	0.84993	1.27967	0.62634	0.66219	2.07955
8	0.80610	0.85694	1.27143	0.63950	0.65245	2.14681
9	0.79641	0.87597	1.26374	0.65407	0.64484	2.17269
10	0.78811	0.88594	1.25747	0.67253	0.63822	2.23886
11	0.78085	0.90528	1.25144	0.69045	0.63281	2.27586
12	0.77446	0.91906	1.24648	0.71270	0.62799	2.34148

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.24946	0.75028	0.91106	1.26803	1.00098	0.79695
2	1.25014	0.70969	0.84675	1.49739	0.90879	0.86997
3	1.21507	0.64484	0.81759	1.58741	0.80064	1.00480
4	1.17284	0.65393	0.82752	1.61524	0.77240	1.02814
5	1.15861	0.66547	0.80069	1.66650	0.74999	1.03937
6	1.14552	0.67495	0.78959	1.67988	0.72939	1.05078
7	1.13411	0.68569	0.77693	1.73967	0.71293	1.05466
8	1.12470	0.69270	0.76732	1.76364	0.69914	1.07288
9	1.11662	0.70830	0.75859	1.82314	0.68714	1.08012
10	1.10945	0.71805	0.75158	1.85821	0.67753	1.09887
11	1.10350	0.73535	0.74507	1.91872	0.66875	1.10913
12	1.09802	0.74819	0.73982	1.96563	0.66178	1.12803

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.92754	1.39450	0.84705	0.84838	1.33220	0.61684
2	1.01140	1.27327	0.80561	0.91022	1.30317	0.64380
3	1.04363	1.29761	0.75883	0.92283	1.28258	0.63119
4	0.99888	1.35328	0.73858	0.92524	1.27877	0.62500
5	0.99018	1.36618	0.71666	0.93591	1.26571	0.64776
6	0.97223	1.41490	0.70218	0.93931	1.25795	0.65982
7	0.96053	1.43532	0.68843	0.95738	1.24973	0.68189
8	0.94919	1.48421	0.67733	0.96408	1.24333	0.69888
9	0.94045	1.51475	0.66781	0.98283	1.23697	0.72287
10	0.93212	1.56573	0.65958	0.99251	1.23185	0.74643
11	0.92573	1.60681	0.65262	1.01133	1.22668	0.77442
12	0.91947	1.66182	0.64649	1.02472	1.22237	0.80394

WNT= 29 WE= 75.00000 TIME= 5.00000
 PHOT= 0.20000 PHOB= 0.20000 BETA= 1.00000
 YBO= 0.00095 YCO= 0.00086

CONCENTRATION TRANSIENTS IN STAGE 1

	T1		T2		T3	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.95503	0.85810	1.15014	0.72888	1.00000	1.01393
2	0.95456	0.87956	1.15755	0.75049	0.95085	1.19590
3	0.91852	0.84904	1.17310	0.73427	0.87936	1.47587
4	0.90797	0.79024	1.17019	0.70399	0.84011	1.44506
5	0.87420	0.77003	1.15450	0.68096	0.81761	1.40099
6	0.85010	0.76902	1.14607	0.65596	0.80251	1.38870
7	0.86903	0.75935	1.13852	0.65475	0.78680	1.36663
8	0.86083	0.75109	1.13214	0.64090	0.77529	1.35339
9	0.85344	0.74443	1.12700	0.63205	0.76557	1.33975
10	0.84737	0.73971	1.12277	0.62323	0.75753	1.32952
11	0.84234	0.73479	1.11925	0.61670	0.75093	1.32022
12	0.83818	0.73111	1.11637	0.61081	0.74548	1.31275

CONCENTRATION TRANSIENTS IN STAGE 2

	T2		T3		T1	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	1.15255	0.79920	0.96222	1.22518	1.02122	0.82923
2	1.15554	0.75906	0.92007	1.35262	0.99167	0.82734
3	1.14217	0.70795	0.87381	1.40830	0.96433	0.81574
4	1.12324	0.67971	0.86158	1.35091	0.95199	0.80329
5	1.11374	0.66157	0.84436	1.33809	0.93117	0.79121
6	1.10267	0.65061	0.82894	1.30810	0.91921	0.77978
7	1.09496	0.63807	0.81688	1.29228	0.90847	0.77245
8	1.08845	0.63021	0.80651	1.27404	0.89946	0.76490
9	1.08305	0.62218	0.79804	1.26130	0.89219	0.75953
10	1.07863	0.61637	0.79105	1.24916	0.88612	0.75454
11	1.07493	0.61105	0.78527	1.23972	0.88110	0.75066
12	1.07196	0.60687	0.78049	1.23135	0.87695	0.74726

CONCENTRATION TRANSIENTS IN STAGE 3

	T3		T1		T2	
M	YA1/YA0	YB1/YB0	YA2/YA0	YB2/YB0	YA3/YA0	YB3/YB0
1	0.97400	1.31603	0.94586	0.82175	1.18658	0.71426
2	1.00274	1.25636	0.93937	0.82034	1.15396	0.76654
3	1.00841	1.23846	0.91669	0.80370	1.11683	0.77741
4	0.97505	1.23441	0.89643	0.78290	1.10709	0.74214
5	0.95900	1.19258	0.88380	0.77376	1.09767	0.72968
6	0.94616	1.17724	0.86988	0.76542	1.08981	0.70896
7	0.93413	1.15387	0.85996	0.75808	1.08327	0.69777
8	0.92495	1.13983	0.85154	0.75251	1.07793	0.68514
9	0.91724	1.12504	0.84455	0.74749	1.07348	0.67645
10	0.91086	1.11425	0.83881	0.74352	1.06984	0.66820
11	0.90562	1.10429	0.83406	0.74008	1.06682	0.66186
12	0.90128	1.09640	0.83013	0.73726	1.06434	0.65626

NOMENCLATURE

a	surface area for mass transfer
b	dimensionless equilibrium parameter
A,B,D	temperature dependent Langmuir constants (Eq. 4.17)
C	as defined by Eq. 5.30
C_A, C_B	concentration of components A and B (Fig. 5.4)
D_S	solid phase diffusivity
E_D	liquid phase axial diffusivity
H,h	column height, cm
L(T)	penetration distance as a function of temperature
M	x/y, cc/gm
m	dimensionless equilibrium parameter for parapump or equilibrium constant for packed column design (x/y, cc/gm)
n	number of cycles
Q	reservoir displacement rate for parapump (cc/min) or column displacement volume for staged sequence (cc)
v_O	interstitial velocity cm/min
u	solute concentration velocity
p_1	as defined by Eq. 4.87
V_T	top reservoir dead volume, cc
V_B	bottom reservoir dead volume, cc
x	concentration of solute in the solid phase, gm moles/gm of adsorbent
y	concentration of solute in the liquid phase, gm moles/cc

T_1, T_2, T_3	column operating temperatures
P	product volumetric flow rate/reservoir displacement rate for parapump or volume of product/column displacement for staged sequence, dimensionless
t	duration time, mins
r	radius of spherical particle
z	column axis
R_B, R_T, R_I	bottom, top and intermediate reflux ratios
SF	separation factor
<>	average value

Greek Letters

β	reflux ratio or recycle ratio
ϵ	void fraction in packing, dimensionless
ρ_s	density of adsorbent, gm/cc
ρ_f	density of fluid, gm/cc
τ	dimensionless time for adsorption step
τ'	dimensionless time since start of desorption
Δ	change

Subscripts

o	initial condition
B	stream from or to bottom of the column
T	stream from or to top of the column
i	solute i
A, B	solutes A and B
F	stream from feed
n	number of cycle

∞

steady state

B,I,T

bottom, intermediate and top

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