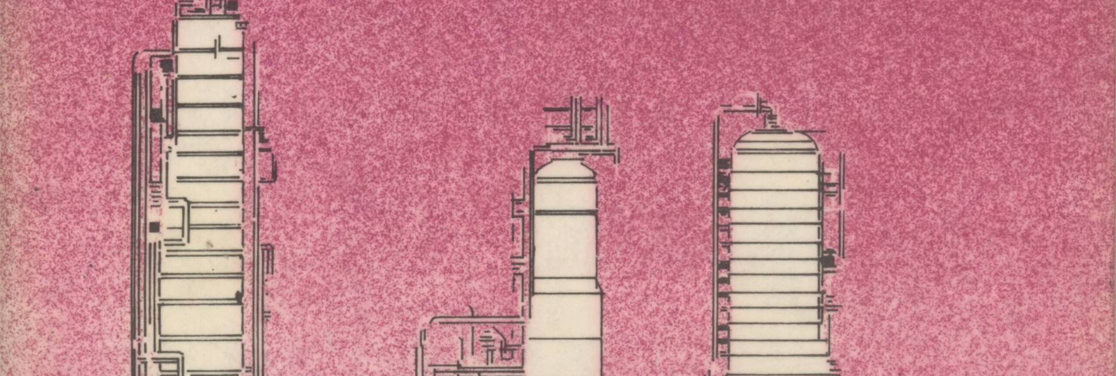
DISTILLATION AND ABSORPTION

1987



European Federation of Chemical Engineering
Europäische Föderation für Chemie-Ingenieur-Wesen
Fédération Européenne du Génie Chimique

EFCE Publication Series No. 62

The
Institution of
Chemical
Engineers

Hemisphere
Publishing
Corporation

Volume 1
PLENARY

EFCE Event No. 352

Distillation and Absorption 1987

A three-day symposium organised by The Institution of Chemical Engineers Fluid Separation Group and the EFCE Distillation, Absorption and Extraction Working Party, and held at the Brighton Centre, Brighton, 7-9 September 1987

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THE INSTITUTION OF CHEMICAL ENGINEERS
SYMPOSIUM SERIES NO 104

ISBN 0 85295 209 0

PUBLISHED BY THE INSTITUTION OF CHEMICAL ENGINEERS

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ISBN 0 89116 840 0 (Set)
ISBN 0 89116 841 9 (Volume 1)
ISBN 0 89116 842 7 (Volume 2)

Preface

Is it not incredible that distillation, a process practised by the ancient Egyptians, still justifies a conference? Surely, it may be argued, everything significant about the subject has already been observed and recorded.

In fact distillation is such a fundamental separation process that, like the structure of the atom, the more one explores the more there is to find. It is fundamental because it depends only on the difference in composition which normally exists between the vapour and liquid phases of the mixture to be separated. It does not require any special solid surface to absorb or sift one of the components, or any additional chemical to react reversibly with it. And for related reasons there is no need for a solid matrix or secondary fluid through which diffusion must occur thereby limiting the rate of separation.

The rates of molecular movement which occur at the vapour-liquid interface are so rapid that even in the most intense distillation processes they exceed the separation flux by a factor of much more than a hundred. That is why the centrifugal field used in Hygee devices could concentrate the separation into such a small volume. The limiting rate of separation we can achieve in distillation is limited only by our ingenuity in achieving controlled turbulence on either side of the interface whilst moving the phases countercurrently. It is this enormous *rate* of separation achieveable in distillation which guarantees its use for centuries to come.

On this occasion we have spread our wings to embrace absorption as well. I believe this is a wise move since so much of the theory and hardware of distillation and absorption are shared. But it is useful also to recognise the difference. Absorption is much more restricted in application, and it is much slower. It is restricted to the separation of gaseous mixtures, and normally to those in which the soluble component is relatively dilute. It is slower because there is always much inert gas through which the soluble component has to diffuse. If the solubility is low there will need to be plenty of interfacial area or high turbulence in the phases. So absorption also provides a challenge to ingenuity.

My judgement is that distillation and absorption will be advanced but not exhausted in 1987.

Geoffrey Haselden

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A NEW NUMERICAL SCHEME FOR ABSORBERS AND DISTILLATION COLUMNS - CINEMATIC MODELLING

C. Lakshmanan* and O.E. Potter**

Most existing numerical methods are not able to describe adequately the effect of disturbance(s) on the dynamic behaviour of countercurrent systems due to the advective nature of these systems. This paper reports a new numerical model - the 'Cinematic' - a model which enables a rapid and accurate computation of a variety of situations commonly encountered in chemical process industries. Examples considered include tray absorbers and tray distillation columns with linear and nonlinear equilibrium relations.

INTRODUCTION

To simulate the dynamic behaviour of countercurrent systems, Lakshmanan and Potter (1984) have developed a new numerical model, namely, 'Cinematic' model. This model has been applied successfully to a number of dynamic simulation problems including double pipe heat exchangers, plate heat exchangers, packed gas absorbers and gas-solid fluidised beds. Based on these numerical experiments, it has been found that this model is computationally fast and accurate. Also, problems usually encountered by other numerical schemes, such as convergence and inversion of results from transformed domain to time domain etc. are not encountered in using the 'Cinematic' model. The problem of obtaining the dynamic response becomes increasingly difficult when the system under consideration has severe nonlinearities. Therefore, in this paper the 'Cinematic' model is applied to linear and nonlinear gas absorption and binary distillation in tray type columns.

APPLICATION OF THE 'CINEMATIC' MODEL TO GAS ABSORPTION

Prior to the disturbance, solute free gas and liquid flow through the column. At t = 0, a step increase in the solute concentration of the gas entering the absorber is effected. The 'Cinematic' model is applied to simulate the dynamic response of the absorber until steady state is attained.

The calculations involved in using the 'Cinematic' model consists of two major steps namely, the mixing step and the mass transfer step. The sequence in which these two steps are applied to a particular problem differentiates between the two approaches of processing, namely the forward and reverse processing.

In applying the 'Cinematic' model to the gas absorption problem, the following assumptions are made. They are:

1. The absorber is assumed to be operating under isothermal conditions.
2. Perfect mixing is assumed in both gas and liquid phases.
3. Each tray is assumed to be an ideal state.

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4. On each tray, the exchange of solute between the two phases are assumed to be taking place at equilibrium.

5. The gas and liquid hold-ups in each tray are assumed to be constant.

Forward processing:

In this mode of processing, the mixing step takes place first followed by the mass transfer step. The mixing step is considered to be infinitely fast. A quantum of liquid is defined as a fraction of the liquid held on a tray. This quantum, QH_L, of the liquid entering the absorber is added to the top tray and the added quantum trickles through all trays and exits at the liquid outlet. As a result of this mixing step, the concentration of liquid phase in each tray changes. As perfect mixing is assumed in the liquid phase, the new set of liquid phase concentrations in every tray can be calculated using the equation given by Mason and Piret (1950). If x_{j0} is the initial concentration of solute in the liquid on tray j before the addition of the quantum and x_0 is the concentration of the solute in the liquid quantum added, then the new set of concentrations can be given by:

$$x_n = x_0 + e^{-Q} \sum_{j=1}^{n} \frac{(x_{j0} - x_0)}{(n-j)!} Q^{(n-j)} \quad \text{for } n=1,2,....N \tag{1}$$

x_n is the concentration of the solute in the nth tray after the mixing step. The time interval Δt, for the mixing step is equal to QH_L/L_M where L_M is the molal rate of flow of liquid entering the absorber. The liquid leaving the absorber is given by the time averaged value $\bar{x}_N$ calculated as:

$$\bar{x}_N = \frac{1}{\Delta t} \int_0^{\Delta t} x_N \, dt \tag{2}$$

Using equation (1), the integral in equation (2) can be evaluated and the average concentration $\bar{x}_N$ can be given as,

$$\bar{x}_N = x_0 + \frac{1}{\Delta t} \int_0^{\Delta t} e^{-Pt} [I_0 + I_1 t + I_2 t^2 + \dots I_{N-1} t^{N-1}] \, dt \tag{3}$$

where, $P = L_M/H_L$ and $I_{N-j} = \frac{(x_{j0} - x_0)}{(N-j)!} P^{(N-j)}$ for $j=1,2...N$

The integration in equation (3) is performed analytically. The mixing step is now complete and the mass transfer step begins. The mass transfer step is considered to be taking place during all of the time interval Δt. In this step, a quantum of gas appropriate to the liquid feed quantum is introduced at the gas inlet. In other words, this quantum of gas is equal to $\Delta t \, G_M$. Let $\bar{y}_{n+1}$ be the time averaged mole fraction of solute in gas leaving (n+1)th tray. A differential mass balance can be written for the transfer of solute between the two phases as

$$H_L \frac{dx_n}{dt} = G_M (\bar{y}_{n+1} - y_n) \tag{4}$$

and the mole fraction y_n of the solute in gas leaving tray n can be given by integrating equation (4) as ,

$$y_n = \bar{y}_{n+1} - (\bar{y}_{n+1} - y_{n,0}) \exp(-QmG_M/L_M) \tag{5}$$

where $y_{n,0}$ is the mole fraction of the solute in gas on tray n at the beginning of the mass transfer step. Note that this ignores the hold-up in the gas phase dispersed in the liquid. The time averaged mole fraction of the solute in gas leaving tray n can be given by,

$$\bar{y}_n = \bar{y}_{n+1} - (\bar{y}_{n+1} - y_{n,0})(L_M/mG_MQ) \tag{6}$$

It must be noted that $\bar{y}_{N+1}$ equals y_0, the inlet gas composition. Equations (4) to (6) are valid only when the absorption equilibrium is linear ($y^* = mx$). Nonlinear equilibrium will be considered later. Using equations (1) to (6), the sequence of calculations that needs to be coded into a computer programme is given next.

Algorithm for forward processing

a)Input number of trays, gas and liquid phase flow rates, the equilibrium relation and the mole fraction of solute in the feed gas.

b)Initialise the gas and liquid phase compositions in all trays.

c)Choose a quantum size.

d)Begin the mixing step.

e)Calculate the new set of liquid phase compositions for all trays using equations (1) and (2).

f)Calculate the time averaged composition of the liquid leaving the absorber using equation (4).

g)Introduce an appropriate quantum of gas at the gas inlet.

h)Calculate the gas and liquid phase compositions after the transfer step for all trays.

i)Calculate the composition of gas leaving the absorber.

j)Reinitialise the gas and liquid phase composition for all trays.

k)Repeat steps (c) to (j) until steady state is attained.

Algorithm for reverse processing

In this approach, a quantum of gas is introduced first and the calculations are performed for the mass transfer step. Then an appropriate quantum of liquid is introduced at the top of the absorber and the mixing step is commenced. The sequence in which the calculations are to be performed are given next.

a)Initialise the gas and liquid phase compositions in every tray.

b)Introduce a quantum of gas at the gas inlet.

c)Calculate the gas and liquid phase compositions after the transfer step for all trays using equations (5) and (6).

d)Calculate the composition of gas leaving the absorber.

e)Begin mixing step by introducing an appropriate quantum of liquid at the liquid inlet.

f)Calculate new set of liquid phase compositions on trays after the mixing step using equation (1).

g)Calculate the composition of liquid leaving the absorber using equation (3).

h)Reinitialise the gas and liquid phase compositions on each tray.

i)Repeat steps (b) to (h) until steady state is established.

EXAMPLE

Consider a tray absorber through which solute free liquid and gas flow initially. At $t=0^+$, the concentration of the incoming gas is stepped up to a particular value. The required data is given below.

Data: Number of trays =6; Flow rate of liquid=40.8 kmol/min; Flow rate of gas=66.7 kmol/min; $y^* = mx = 0.72x$; $H_L = 75$ kmol per plate; $H_G = 1$ kmol per plate; Liquid entering is solute free; At $t=0^+$, mole fraction of solute in the feed gas is increased to 0.3.

Calculations are performed using both forward and reverse approaches of the 'Cinematic' model until steady state is achieved. The results are also compared with the results obtained using the analytical solution given by Douglas (1972). The results of the simulations indicated that the reverse approach is preferred when the disturbance to the system enters only through the entering gas. Simulations performed with various quantum sizes (0.05, 0.2, 0.5, 1.0) indicated that quantum sizes 0.05, 0.2 and 0.5 produced identical results. The results are shown in figures (1) and (2).

NONLINEAR EQUILIBRIUM

Consider absorption of sulfur dioxide in water in a tray absorber with the following operating conditions. The carrier gas is air.

$N=13$; $L_{SM}=1891.39$ kmol/h; $G_{MB}=30$ kmol/h; $H_L=5.56$ kmol absorbent per plate; Gas hold-up is neglected. Prior to the disturbance, solute free air and water flow through the absorber and at $t=0^+$, the solute concentration is stepped up to 0.5 kmol solute/kmol carrier gas in the feed. The 'Cinematic' model is then used to simulate the approach to steady state of this system. The following equilibrium relations are fitted.

$$y = a_1x + a_2x^2 + a_3x^3 + a_4x^4 \qquad \text{for } 0 \leq x \leq 0.000422$$

$$y = b_0 + b_1x + b_2x^2 + b_3x^3 \qquad \text{for } x > 0.000422$$

It must be noted that these equilibrium relations use mole fractions of the solute in gas and liquid. The constants are:

$a_1=14.37$; $a_2=-65454.04$; $a_3=0.3696$ E+09; $a_4=-0.4591$ E+12

$b_0=-0.4091$ E-02; $b_1=27.689$; $b_2=425.496$; $b_3=-6936.947$

It may be recalled from the results obtained for the linear equilibrium case that reverse approach produces the least error for a start-up problem such as the one considered here. Hence, for the nonlinear equilibrium case, calculations are shown only for reverse processing.

Firstly, the mixing step is performed as described before. The new set of concentrations are given as:

$$C_n = C_0 + e^{-Q}\sum_{j=1}^{n}\frac{(C_{j,0} - C_0)}{(n-j)!}Q^{(n-j)} \qquad \text{where } Q = \frac{L_{SM}}{H_L}\Delta t \tag{7}$$

This calculation is repeated for all n from 1 to N. The concentration of liquid leaving the absorber $\bar{C}_N$ is calculated as:

$$\bar{C}_N = \frac{1}{\Delta t}\int_0^{\Delta t} e^{-Pt}\left[I_0 + I_1t + I_2t^2 + \ldots I_{N-1}t^{N-1}\right]dt \tag{8}$$

where, $P = L_{SM}/H_L$ and $I_{N-j} = \dfrac{(C_{j0} - C_0)}{(N-j)!}P^{(N-j)}$ for $j=1,2\ldots N$

From the data given, it can be inferred that the equilibrium and the operating line are curved. Since the molar density of the liquid changes through the column, the mole fraction of the solute in the liquid over trays after the mixing step is calculated from the molar concentrations using the following relation.

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$$x_n = \frac{18C_n}{18C_n + 1} \tag{9}$$

For the transfer of solute which takes place for a differential time Δt, the following mass balance can be written

$$\frac{dx_n}{dt} = (1-x_n)^2 \frac{G_{MB}}{H_L}\left[\frac{\bar{y}_{n+1}}{(1-\bar{y}_{n+1})} - \frac{y_n}{(1-y_n)}\right] \tag{10}$$

Since the equilibrium relation is highly nonlinear, the result of the transfer step cannot be given in a closed form. It may also be noted that equation (10) uses G_{MB} instead of G_M as the gas velocity changes significantly between the inlet and the outlet for the problem chosen. Equation (10) together with the nonlinear equilibrium sets up an initial value problem which is highly nonlinear. The solution is obtained using the routine **DGEAR** of the IMSL (1982). The numerical solution is carried out until t=Δt to give the mole fraction of the solute in the liquid phase after the transfer step. Corresponding gas phase mole fraction is obtained using the equilibrium relation. The time averaged mole fraction of the solute leaving tray n is obtained from an overall mass balance around tray n given by,

$$\bar{Y}_n = \bar{Y}_{n+1} + H_L\left[\frac{x_{n,0}}{(1-x_{n,0})} - \frac{x_{n,1}}{(1-x_{n,1})}\right]\frac{1}{G_{MB}\Delta t} \tag{11}$$

and $\bar{y}_n$ can be calculated as $\frac{\bar{Y}_n}{1+\bar{Y}_n}$.

Algorithm

a)Input G_{MB}, L_{SM}, H_L, H_G and N

b)Choose quantum size Q.

c)Initialise the mole ratio's of the solute in gas and liquid phases on all trays.

d)Commence the mixing step by introducing the quantum of liquid at the top of the absorber.

e)Calculate the new set of compositions in the liquid phase using equations (7) and (8).

f)Calculate the time averaged composition of the liquid leaving the absorber using equation (9).

g)Begin the mass transfer step by introducing an appropriate quantum of gas at the gas inlet.

h)Calculate the compositions after the transfer step using equations (10) and (11).

i)Calculate the time averaged composition of the gas leaving the absorber using equation (11).

j)Reinitialise the compositions of gas and liquid phases.

k)Repeat steps (d) to (j) until steady state is established.

NUMERICAL SOLUTION USING GEAR's ALGORITHM

Assuming perfect mixing in both gas and liquid phases the dynamic mass balance for nth tray can be written as:

$$H_G\frac{dY_n}{dt} + H_L\frac{dX_n}{dt} = L_{SM}(X_{n+1}-X_n) + G_{MB}(Y_{n-1}-Y_n)$$

If the gas hold-up is neglected as being insignificant the mass balance can be rearranged to give,

$$\frac{dx_n}{dt}=\frac{L_{SM}}{H_L}(1-x_n)^2\left[\frac{x_{n+1}}{1-x_{n+1}}-\frac{x_n}{1-x_n}\right]+\frac{G_{MB}}{H_L}(1-x_n)^2\left[\frac{y_{n-1}}{1-y_{n-1}}-\frac{y_n}{1-y_n}\right] \tag{12}$$

This equation can be integrated for n=1 to N from $t=0^+$ until steady state is established. y_0 is the gas composition at the gas inlet and x_{N+1} is the composition of the liquid entering the column. The integration is performed using **DGEAR** subroutine of IMSL(1982) and the results are plotted in figures (3) and (4) along with the results obtained from the 'Cinematic' model. It can be seen that the two results agree well. The results shown in figures (3) and (4) correspond to a quantum size (Q)=0.2. Figure (5) shows the effect of quantum size on the error introduced in steady state recovery. The error in recovery is defined as shown:

$$\text{The \% error in recovery for the gas phase}=100\,\frac{\bar{Y}_1(Q=0.2)-\bar{Y}_1(Q)}{1.-\bar{Y}_1(Q=0.2)}$$

$$\text{The \% error in recovery for the liquid phase}=100\,\frac{\bar{X}_N-\bar{X}_N(Q=0.2)}{\bar{X}_N(Q=0.2)}$$

In calculating these errors, Q=0.2 is chosen as the reference since the simulated results with this quantum size agreed perfectly well with the numerical solution produced by using **DGEAR**. The mole ratios used in the recovery calculations are the outlet mole fractions of the two phases.

In the case of nonlinear equilibrium, the number of trays in the absorber is varied and the dynamic simulations are performed using the 'Cinematic' model and **DGEAR**. The dynamic profiles are shown to be in good agreement with each other as shown in figures (6) and (7). It is interesting that a change in number of trays has a significant influence on the rate of approach to steady state of the gas phase but has not affected the rate of approach of the liquid phase. Increasing the number of trays increases the residence time of the gas phase in the absorber. But the observed delay in approaching steady state for the gas phase is more than the increase in residence time that can be accounted as due to the additional trays. To find out if this behaviour is a characteristic of the nonlinear equilibrium, similar calculations are performed for the linear equilibrium as well. The results shown in figure (8) indicate that increasing number of trays increases the time required to attain steady state even for the linear equilibrium.

From the analytical solution for a tray type gas absorber, time required to attain equilibrium, can be calculated as a function of the number of trays, N. Marshall and Pigford (1952) have defined the degree of approach to equilibrium as the difference between the driving force at the top of the column at equilibrium and the instantaneous driving force and plotted this rate of approach versus number of theoretical stages using the absorption factor as a parameter. From their graph, it can be seen that a delayed approach to steady state is possible. Jackson and Pigford (1956) carried out a similar study. It may be noted that the problems solved by them are either linear or a linearised nonlinear problem. As obtaining an analytical solution for a nonlinear problem such as the one considered in this work is not possible, a plot similar to the one given by Marshall and Pigford can be constructed only from a variety of accurate numerical solutions which further justifies the need for an accurate numerical scheme.

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APPLICATION OF THE 'CINEMATIC' MODEL TO DISTILLATION

The method of calculations outlined for tray absorbers can be extended to distillation. As a simple case, consider the start-up of a column at total reflux operating on a binary equi-molar feed which is, at t=0, considered to fill the column hold-up and to be at the bubble-point. Raoult's law and constant molal overflow are assumed. The condenser is assumed to have hold-up, H_C, which is well-mixed.

Operation starts by the vapourisation of a finite quantity of vapour, represented in the calculation as fraction, Q, of the hold-up on an individual tray. The liquid in the reboiler is essentially subjected to a batch distillation. Vapour released is considered to be trapped and well-mixed before flowing to the tray above. Equilibrium is assumed on each tray and in the reboiler. Composition of liquid in the reboiler changes. Vapour from the reboiler, at constant composition, $\bar{y}$, flows through the liquid on tray above and yields a vapour instantaneously in equilibrium with the liquid on the tray. Vapour is considered to be trapped and uniformly mixed before flowing to the tray above. And so on up the column. Vapour leaving the tray at the top is condensed and mixes well with the liquid in the condenser hold-up. The first transfer step is concluded. Now begins the reflux mixing step. This is considered to occur instantaneously. A quantity of reflux, equal at total reflux to the quantity of vapour, flows to the top tray and down the column to the reboiler. Liquid on each tray is well-mixed. Liquid leaving the tray above the reboiler is considered to be trapped and mixed well before flowing to the reboiler, where it restores the liquid hold-up to what it was initially.

The process described above occurs repeatedly. The composition on each tray is followed as time proceeds. A number of calculations have been performed in Basic on an IBM PC AT or a compatible XT. Figure(9) shows the approach to steady state at total reflux for a column consisting of six theoretical stages and a binary mixture of relative volatility 2.5. Notice that quantum sizes, Q, of 0.1 or smaller are indistinguishable on the graph but the large quantum size of Q=1.0 is differentiated at least in the rectifying section. In figure(10) the "per cent error in N" at the steady state as calculated by 'Cinematic' model is portrayed as a function of step-size for a six theoretical stage column with relative volatility of 1.25. From these two figures it can be concluded that a relatively coarse quantum size, Q, can be used to approximately follow the transient but that an accurate calculation of fine deviations from steady state requires a smaller value. The Underwood-Fenske equation applied to the steady state results at different Q values enables an effective number of trays, N_{eff}, to be calculated. The percentage error of N_{eff} with respect to N is plotted.

Figure (11) shows the approach to steady state at long times for a 48-tray column with relative volatility of 1.25 and a 121-tray column with relative volatility of 1.05. "Per cent deviation from steady state" is plotted versus τ where τ is the number of residence-times or more strictly turnovers. τ=1 implies that the vapour generated in the reboiler is equal to the total column hold-up. τ=10 implies ten times this amount of vapour has been generated and passed through the column to the condenser.

SUMMARY

Based on the computations performed, it can be seen that the 'Cinematic' model is easy to use and provides an accurate account of the dynamic behaviour of tray type countercurrent systems. The application of this new model to other countercurremt systems will be reported elsewhere. The computations does not involve any infinite series and therefore the problems such as convergence and numerical stability do not exist. The model is simple and easy to apply and allows the user to perform fast numerical computations. No particular difficulty has been noticed in applying the model to a nonlinear problem.

NOTATION

C_0 -concentration of the solute in liquid entering ,moles/l
C_n -concentration of the solute in liquid on tray n ,moles/l
G_M -flow rate of gas ,moles of solute plus carrier gas/h
G_{MB} -flow rate of gas ,moles of solute free gas/h
H_C -hold-up in condenser of liquid ,moles/h
H_G -hold-up of gas per plate ,kmol for linear equilibrium case only
H_G -hold-up of gas per plate ,kmol on a solute-free basis for nonlinear equilibrium
H_L -hold-up of liquid per plate ,kmol for linear equilibrium case only
H_L -hold-up of liquid per plate ,kmol on a solute-free basis for nonlinear equilibrium
L_M -rate of flow of liquid ,kmol/h
L_{SM} -rate of flow of liquid ,kmol/h solute-free basis
m -slope of equilibrium line
N -number of trays
Q -quantum size ,fraction
Δt -time step
x_0 -mole fraction of solute in liquid entering
x_{jO} -mole fraction of solute on tray j before the mixing step
x_n -mole fraction of solute on tray n after the mixing step
$\bar{x}_N$ -time-averaged mole fraction of liquid leaving the absorber
y -mole fraction of solute in gas
$\bar{y}_{N+1}$ -average mole fraction of solute in gas leaving the absorber
Y -mole ratio, moles solute/moles carrier gas

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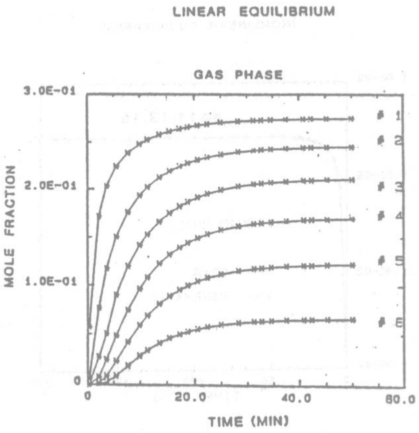


Fig. 1: Dynamic response of a tray absorber

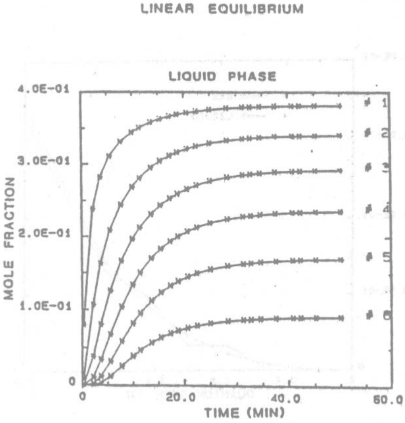


Fig. 2: Dynamic response of a tray absorber

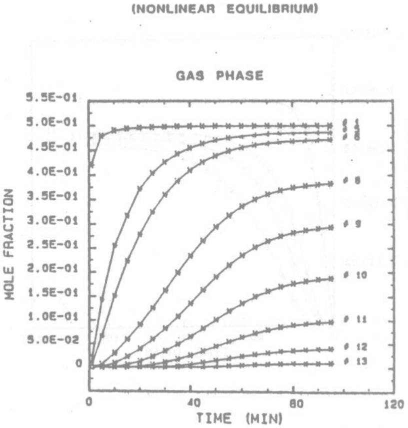


Fig. 3: Dynamics of a tray absorber

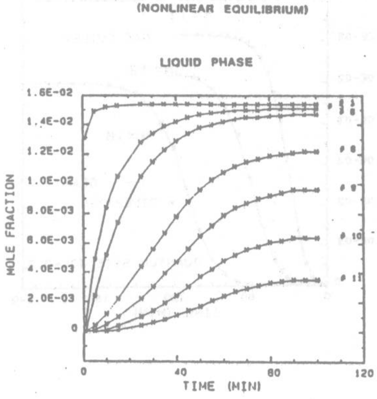
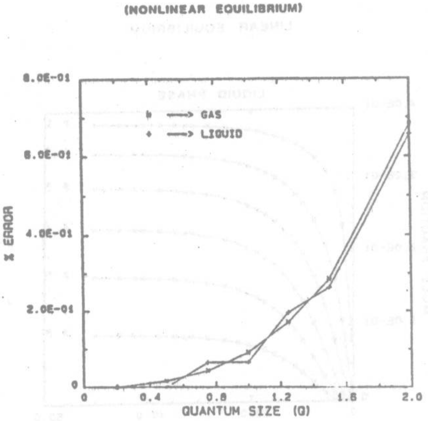


Fig. 4: Dynamics of a tray absorber



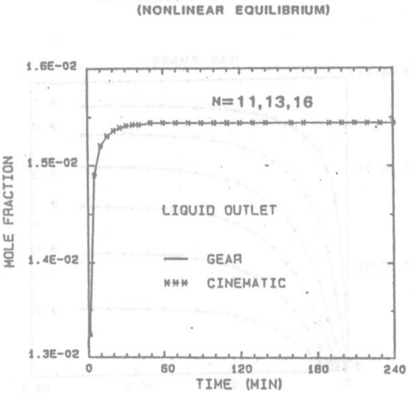
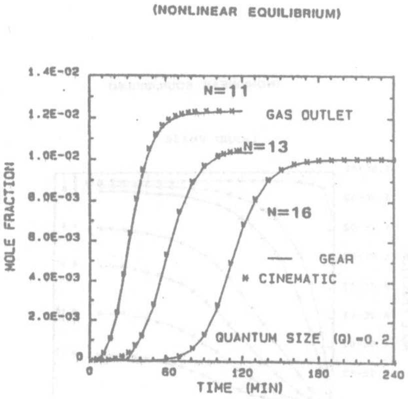


Fig. 5: Effect of quantum size on the recovery (steady state)

Fig. 6: Effect of number of trays on the approach to steady state



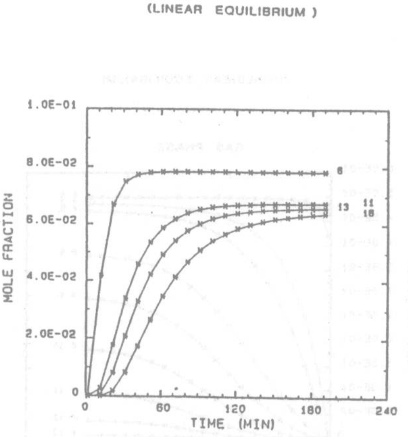


Fig. 7: Effect of number of trays on the approach to steady state

Fig. 8: Effect of number of trays on the approach to steady state

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