

DISTILLATION AND ABSORPTION 1987



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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 achievable 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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MICROCOMPUTER SIMULATION OF DISTILLATION COLUMN OPERATION AND CONTROL

P L Yue* and P J Billing**

The dynamic simulation of the operation and control of a binary distillation column presented in this paper is included as part of an Open Learning course for teaching the principles of distillation to inexperienced process plant personnel who are unfamiliar with distillation. The separation of acetone and ethanol at steady state and the dynamic effects of changing process parameters such as column feed rate and boil-up rate are simulated. Control of the distillation column is achieved by proportional and integral control of the distillate rate and the column bottoms level. The simulation is highly interactive and the Open Learning approach adopted has been shown to be an effective training method which could lead to improvement in the efficiency of the plant personnel¹.

INTRODUCTION

The current rapid advance of computer technology in the 1980's has accelerated the use of microcomputer based systems as plant operation simulators. One important aspect of process plant operation is the efficiency of the plant personnel. Their knowledge and skill can be improved through the use of interactive computer-based-training (CBT). This paper describes a dynamic simulation of the operation and control of a continuous binary distillation column. The simulation was developed to be included as part of an Open Learning course on distillation being produced by Nobel's Explosives Co Ltd at their Stevenston plant in Scotland.

DISTILLATION SYSTEM

The distillation column control system chosen by Stevenston plant personnel is shown in Figure 1. The system consists of a liquid mixture of 80% acetone and 20% ethanol at its bubble point being fed to a plate column with 18 theoretical equilibrium stages. The liquid feedrate to the column is controlled by a proportional + integral action controller. The vapour from the column head is condensed in a total condenser. The liquid distillate flowrate is adjusted by a second P + I controller and this in turn varies the reflux returned to the column. The level of liquid in the column bottom is controlled by a P + I level controller, LC, which opens and closes the bottom product flow control valve accordingly. The bottoms liquid is boiled by heat exchange with saturated steam in an external reboiler. The flow of steam to the reboiler is controlled by a fourth P + I controller.

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A simple control scheme was chosen so that the response of the system could be clearly observed and the desired training objectives achieved. The objectives of the simulation are:

- (a) to show the effect of boil-up rate on column temperatures and product composition
- (b) to show the effect of feedrate on column temperatures and product composition
- (c) to show the effect of reflux ratio on column temperatures and product composition
- (c) to demonstrate the operation of a continuous distillation control system

The student can observe the dynamic effects of changing the process parameters on a series of animated mimic control system displays. These displays were developed to be representative of the style of mimic displays used in modern process control systems³.

The program is written in the high level authoring language called 'USE', and implemented on the Regency microcomputer system⁴. The Regency system was developed specifically for CBT applications. It features a touch-sensitive screen and powerful graphics capability which makes the system ideally suited for high level interactive simulation. The system has been used to produce a number of simulations of chemical plant operation^{2,4,5}.

MATHEMATICAL MODEL

The following assumptions will be made in deriving the mathematical model of the operation of the distillation column control system which is based on similar models presented by Deshpande⁶ and Wei⁷:

- (a) vapour hold-up is negligible
- (b) liquid and vapour are well mixed on each tray
- (c) tray effluent streams are in thermodynamic equilibrium
- (d) column pressure assumed constant
- (e) thermal capacity of the column and tray is negligible
- (f) tray thermal dynamics are assumed to be rapid so that the energy equation reduces to an algebraic equation
- (g) tray efficiency is constant
- (h) thermal dynamics of reboiler and condenser are assumed to be negligible
- (i) reboiler hold-up is negligible compared to column bottom

Consider the schematic diagram of the distillation column in Figure 2. This is based on the assumptions and simplifications listed above and shows the tray numbering system.

Considering the reboiler, ordinary differential equations can be written to describe the variation of the total and component bottoms liquid hold-up:

$$\frac{dM_r}{dt} = L(1) - B - V_r \quad (1)$$

$$\frac{dXMr}{dt} = X_a(1) * L(1) - X_r * B - Y_r * V_r \quad (2)$$

where M_r = total liquid molar hold-up in column bottom
 XMr = acetone liquid molar hold-up in column bottom
 $L(1)$ = total liquid molar flowrate from first tray
 $X_a(1)$ = acetone liquid mole fraction from first tray
 B = bottoms liquid molar flowrate

X_{ar} = bottoms acetone liquid mole fraction
 V_r = total vapour molar flowrate from reboiler
 Y_{ar} = acetone vapour mole fraction from reboiler

The bottoms liquid molar flowrate is dependent on the amount of hold-up in the column bottom as follows:

$$B = 1C_v * \sqrt{M_r} \quad (3)$$

where $1C_v$ = bottoms liquid flow control valve coefficient.

The new bottoms acetone liquid mole fraction can then be calculated from:

$$X_{ar} = X_{Mr}/M_r \quad (4)$$

Using equilibrium y-x-T relationships determined from empirical data for the fixed column pressure, reboiler temperature T_r and vapour composition Y_{ar} can be evaluated. The heat load on the reboiler, Q_r , is dependent on the steam molar flowrate, S :

$$Q_r = S * H_{vap} \quad (5)$$

where H_{vap} = latent heat of vaporisation of saturated steam at 2 atm, 120°C.

The steam molar flowrate is obtained from:

$$S = sC_v * \sqrt{(P_{s1} - P_{s2})} \quad (6)$$

where sC_v = steam flow control valve coefficient,
 P_{s1} = steam supply pressure
 P_{s2} = steam pressure in reboiler

The new total vapour molar flowrate, V_r , returned to the column from the reboiler can be determined from an enthalpy balance over the column bottom.

$$V_r = \frac{L(1) * h(1) - B * h_b + Q_r}{H_r} \quad (7)$$

where $h(1)$ = specific enthalpy of liquid from first tray
 h_b = specific enthalpy of bottoms liquid
 H_r = specific enthalpy of vapour from reboiler

A series of ordinary differential equations is written to describe the variation of the total and component tray liquid hold-up. For the i th tray,

$$\frac{dM(i)}{dt} = L(i+1) + V(i+1) - L(i) - V(i) \quad (8)$$

$$\frac{dX_M(i)}{dt} = X_a(i+1) * L(i+1) + Y(i+1) * V(i+1) - X_a(i) * L(i) - Y_a(i) * V(i) \quad (9)$$

where $M(i)$ = total liquid molar hold-up on i th tray
 $X_M(i)$ = acetone liquid molar hold-up on i th tray
 $L(i)$ = total liquid molar flowrate from i th tray
 $X_a(i)$ = acetone liquid mole fraction from i th tray
 $V(i)$ = total vapour molar flowrate from i th tray
 $Y_a(i)$ = acetone vapour mole fraction from i th tray

An additional term related to the feed is added to the right hand side of the

equations to describe the feed tray. The total molar feed flowrate F is given by:

$$F = fC_v \sqrt{Pf_1 - Pf_2} \quad (10)$$

where fC_v = feed flow control valve coefficient

Pf_1 = feed supply pressure

Pf_2 = column pressure

The acetone liquid mole fraction from the i th tray can be calculated from:

$$X_a(i) = X_M(i)/M(i) \quad (11)$$

The liquid molar flow rate from the i th tray can be calculated using a modified Francis Weir equation:

$$L(i) = C_1 \{M(i) - C_2\}^{1.5} \quad (12)$$

where C_1 and C_2 are constants.

The vapour molar flowrate from the i th tray is evaluated from a tray enthalpy balance:

$$V(i) = \frac{V(i-1) * M(i-1) + L(i+1) * h(i+1) - L(i) * h(i)}{H(i)} \quad (13)$$

where $h(i)$ = specific enthalpy of liquid from i th tray

$H(i)$ = specific enthalpy of vapour from i th tray

Equations (8) to (13) are solved for each tray. Tray temperature and acetone vapour mole fractions are calculated using the empirical equilibrium relationships. The equations must be adjusted to account for the feed when the calculations reach the feed tray.

Finally for the total condenser, the material balances will include the distillate molar flowrate D which is dependent on the condenser hold-up Mc :

$$D = dC_v \sqrt{Mc} \quad (14)$$

where dC_v = distillate flow control valve coefficient.

Similarly, the liquid reflux is given by:

$$L(19) = cC_v \sqrt{Mc} \quad (15)$$

where cC_v = condenser discharge coefficient.

The simulation requires an initial estimate of tray temperature, liquid flow-rate and acetone mole fraction profiles. The estimates were obtained by using a steady state material and energy balance package, 'ChemCAD'. Routines have also been written for a P + I controller and to obtain discharge coefficients for the flow control valves.

DISCUSSION

A sample of the continuous binary distillation control program screen displays as seen by the student are given in Figures 3 to 5. The animated mimic control panel displays were developed to be representative of the style of computer displays used in modern process control systems³.

Figure 3 shows the main process diagram display. It features a diagram of the plant equipment with the values of the measured and controlled variables displayed at the appropriate points. At the bottom of the display there are touch panel boxes which allow the student to change the mode of operation, either manual or automatic of each controller. He can also change the controller setpoint if operating in automatic mode and the valve position if operating in manual mode. For example, if the student wishes to change the feedrate setpoint, he first of all touches the feedrate controller box displayed on the screen. Then he can select the magnitude of the desired change by touching one of the option boxes which will be displayed for that particular controller. The student can obtain help on operating the simulation at any time by pressing the 'help' key and he can also switch to one of two other mimic control panel displays.

Figure 4 shows the controller display which features bar charts of the controller setpoints compared to the current measured values of the controlled variables. The current mode of operation of each controller is also displayed. The third mimic control panel display is shown in Figure 5. This shows the variable trend display which presents the variation of four of the main process variables with time.

Figures 3 to 5 show the effect of a step change in boil-up rate by changing the steam fed to the reboiler. The variable trend display in Figure 5 shows that the acetone concentration in the bottom product steadily decreases as the boil-up rate increases together with an associated rise in bottoms temperature.

The mathematical model used in the simulation is based on a number of simplifications in order to achieve a practical implementation for training purposes without sacrificing realism. For example, it is more important that the model exhibits a high degree of robustness rather than a high degree of mathematical accuracy.

CONCLUSIONS

An interactive microcomputer simulation of a continuous binary distillation column has been developed for the initial training of plant personnel who are unfamiliar with distillation. Computer simulation allows students to observe and practise with a process system in a way which would be costly and dangerous if not impossible on a real plant. The training can be private, to allow students to ask and answer questions and 'teach themselves' without embarrassment at their own pace. The simulation is highly interactive with the student assuming an active role which has been proved to be optimal for learning.

The same methodology can be applied to simulate multi-component systems. However, as the number of variables increases, it will be vital to adopt the most efficient algorithm for solving the equations and mathematical accuracies will also become more important.

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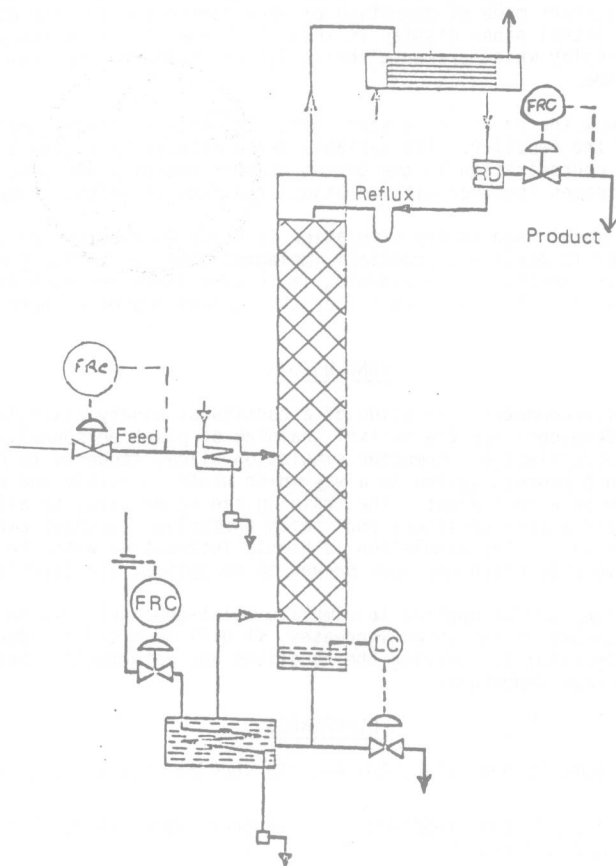


Figure 1 Distillation column control system

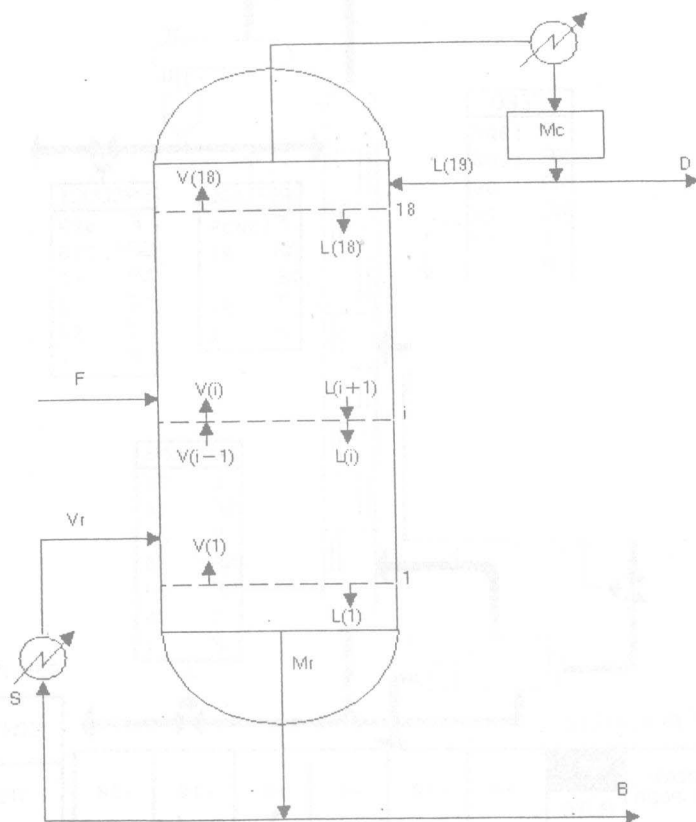


Figure 2 Schematic diagram of distillation column

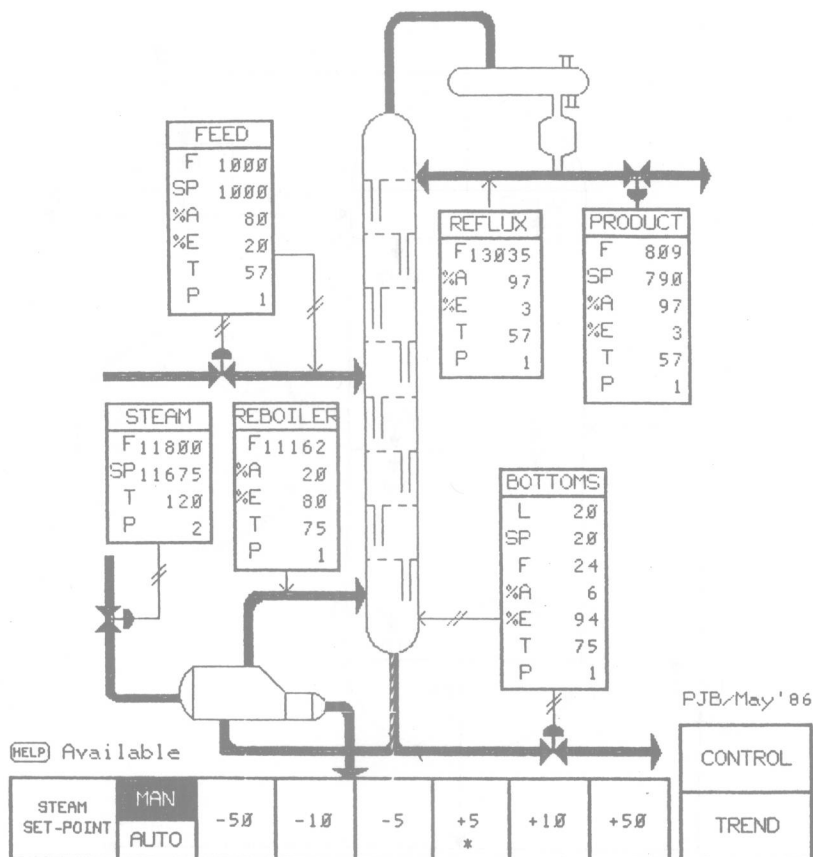
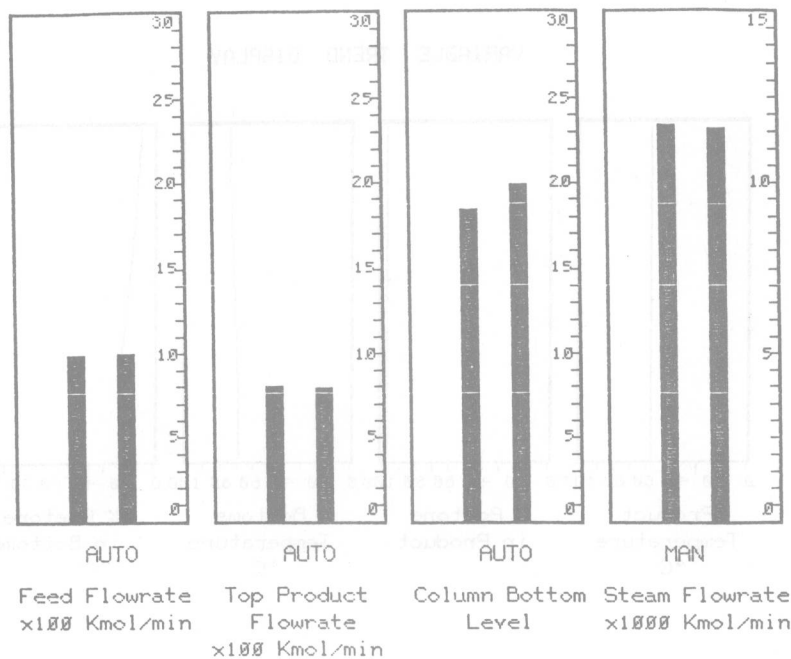


Figure 3 Process diagram display

CONTROLLER DISPLAY

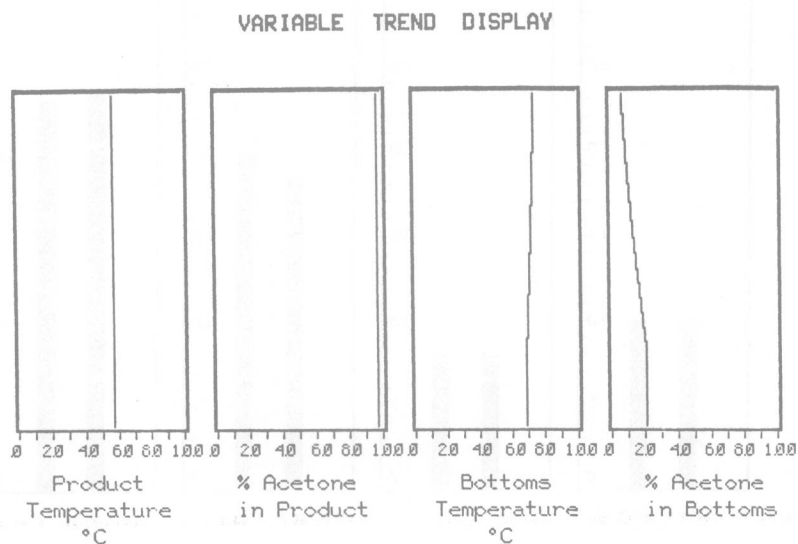


HELP Available

PROCESS

TREND

Figure 4 Controller display



HELP Available

PROCESS

CONTROL

Figure 5

Variable trend display