Multicomponent Distillation Simulation — Distillation of Air

This paper describes the application of a mathematical model to a column distilling air to produce nitrogen, oxygen, and argon. The upper column of a plant producing 400 tonnes/day (400 Mg/day) of oxygen is considered. Apart from any direct interest in this system, the outcome illustrates the problems which arise in the study of the separation of multicomponent systems. The effect of directed flow compared with normal flow is established, and in particular the way in which some components benefit more than others. The simulation uses experimental values of point efficiency and mixing measurements, and a good comparison with plant experience is achieved.

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SCOPE

This paper describes an extensive theoretical study of a distillation column separating air into nitrogen, oxygen, and argon. The column under consideration is the upper column of a plant producing 400 tonnes/day of oxygen.*

The objectives of the study were twofold. First, to use measured values of point efficiency and mixing measurements to mathematically simulate this column, and second, to illustrate the application of the mathematical model to multicomponent separation systems.

The simulation of the column, using the point efficiency measurements made by Haselden and Thorogood (1964), and the author's mixing measurements (Biddulph, 1975) resulted in a good comparison with plant experience. The eddy diffusion model was used. In addition, other values of point efficiency obtained by Brown and England (1961) were used, and various column configurations and conditions studied. These included the effect of vapor mixing, the advantages of directed flow compared with normal flow, and the predicted effect on efficiency of split flow trays.

In the more general objective of studying the simulation of multicomponent separations, the difficulties in attempting to apply correlations based on binary studies are noted.

CONCLUSIONS AND SIGNIFICANCE

A mathematical model has been used to simulate the steady state operation of an air separation column. The simulation of the column using the conditions which were probably closest to those in practice resulted in a column having 60 trays. This compares well with the figures given by Latimer (1967). This simulation used the measured point efficiency values of Haselden and Thorogood (1964). These point efficiencies showed the characteristic fall towards low nitrogen concentrations which has also been noted by other workers. The point efficiency results of Brown and England (1961) were also used, these showing a much more severe fall in point efficiency. The resulting simulation indicated a column having 115 trays, which is much more than practice indicates. This leads to the conclusion that the very severe falls in point efficiency found by Brown and England are not in fact found on commercial operating trays. This is probably due to the fact that the column used was not representative of the conditions at a point on a large tray. The fact that Haselden and Thorogood used a foam baffle above the outlet weir to simulate a point on a large tray may have been an important factor.

The effect of directed flow, that is, liquid flow in the same direction on successive trays, was compared with normal flow. This resulted in a reduction of 3 trays in the column size. In multicomponent systems, the effect is not the same for all the components.

The effect of changing the column to a split flow configuration resulted in 6 extra trays being required. The work of Lim et al. (1974) has indicated that the penalty may not be as great as this.

The effect of vapor mixing has been found, as in other earlier studies of distillation, to be a minor one, changing the column size by 3 trays.

An oscillating efficiency effect has been observed, giving rise to the efficiency going up and down on successive trays. This is only observed in the normal flow regime, and is caused by the composition profiles combining to cause alternate flattening and steepening of the vapor composition profile. This is a minor effect, not present in directed flow.

Distillation is a vital part of many industrial processes. Research and development continues in the general area of distillation in spite of the large amount of work which has been carried out over a period of many years. Zuiderweg (1973) has recently estimated that these activities

* One tonne is equivalent to one megagram or 10^3 kg.

have resulted in savings of possibly $2000 M over the last twenty years.

The recent development of large, high speed digital computer systems has made possible the use of tray models which were formerly too complex for convenient use. This paper is intended to illustrate the application of a simulation model to large commercial columns distilling multicomponent systems. The model uses experimental point efficiency data and a mixing model in both phases. Enthalpy differences between components are included. It was felt that the most satisfactory way of illustrating the use of the model was by considering a large commercial column in detail. Details of operating columns are difficult to obtain, but the upper column of an air separation column was chosen since sufficient data have been provided by Latimer (1967). There is a number of reasons which make this column of particular interest. First, many of these columns are in existence and many engineers are involved in their design or operation. Oxygen production in the western world is now at least 200,000 tonnes/day with a total power consumption of about 3 GW. Furthermore, there is a considerable incentive to keep the number of plates in the column to a minimum since the power consumption represents a substantial fraction of the product cost, and the equipment is expensive. Second, the system is a particularly interesting one in as much as argon is a distributed component, appearing in both top and bottom product streams to a noticeable extent. Third, vapor/liquid equilibrium data and a great deal of experimental point efficiency data are available in addition to data on the mixing characteristics on the small hole size sieve trays used (Biddulph, 1975). For all these reasons, the column is considered to be a useful one with which to demonstrate the use of the simulation method and to enable some conclusions to be drawn regarding other multicomponent systems.

Thus a simulation of the upper column of a low pressure air separation plant is described, based essentially on the configuration given by Latimer (1967). A number of different conditions were studied, including the use of different sets of point efficiency data and various column configurations.

PLANT DESCRIPTION

The upper column which is studied is similar to that in the oxygen gas plant described by Latimer (1967) (Figure 3). The plant has argon columns and refrigeration is made with high pressure air or with liquid input. It corresponds with a plant producing about 400 tonnes/day of oxygen.

The upper column splits a partially liquid stream containing 35.8% oxygen into a gas stream containing 99.75% oxygen from the bottom of the column and an almost pure nitrogen gas stream containing 1 ppm oxygen and a small amount of argon from the top of the column. A sidestream containing approximately 12% argon is taken from a suitable point in the column and some of the argon is recovered from this. The majority of this stream is returned to the column just below the sidestream offtake.

A diagram of the column with feeds and sidestreams marked is given in Figure 1. The conditions given here are for those of simulation number 5, see later, and are similar to those resulting from all the simulations.

The column is designed to have a diameter of 2.13 m, and various possible tray configurations and conditions are simulated. The trays are assumed to be of the usual small-hole sieve type normally used in this application.

Further details of the entire plant are given by Latimer (1967). The column operates at a pressure of 1.4 atmospheres.

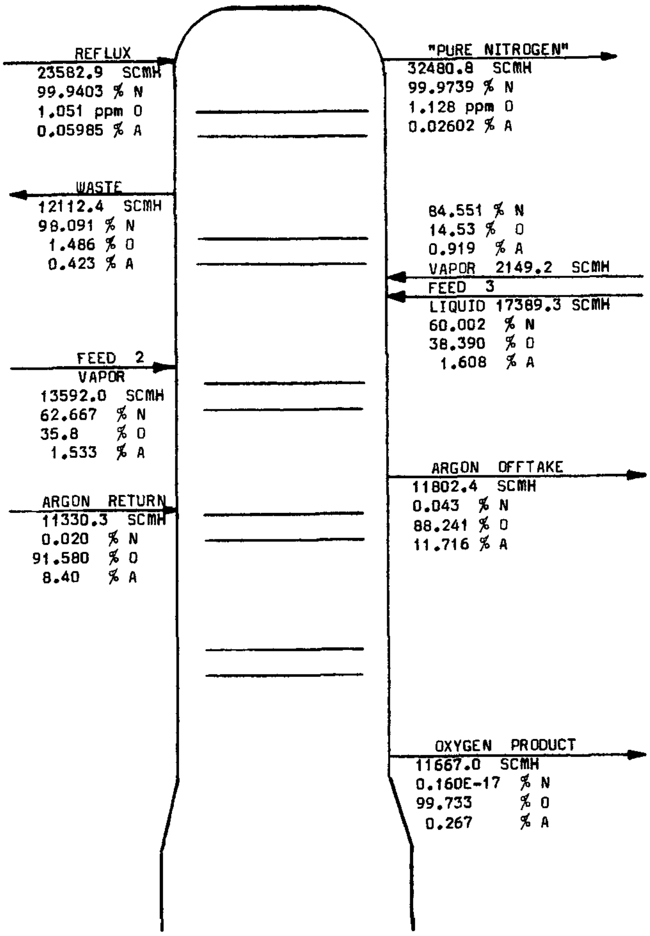

Fig. 1. Column in simulation run 5.

A theoretical stage computer design program for the design of these columns has been described by Armstrong and Schofield (1969), but this of course requires the subsequent application of some value for column efficiency.

CHOICE OF MIXING MODEL

The performance of a distillation column depends on the mixing characteristics both in the biphase on the tray and in the vapor above the biphase. Over a period of many years, a great deal of work has been devoted to the study of mixing and to mathematical models to describe the mixing. A number of models have been proposed, and a choice must be made for use in this simulation. A review of backmixing and design has recently been published by Mecklenburgh (1974).

The models proposed over the years have included the Mixing Pool Model, Recycle Stream Model, Splashing Model, Eddy Diffusion Model, Liquid Residence Time Model, Stagnant Regions Model (Porter et al., 1972; Lockett et al., 1973 and Lim et al., 1974), and Cascade of Cells with Stagnant Zones (Bruin and Freije, 1974).

The eddy diffusion model has been chosen for a number of reasons. It is a convenient model for use in multicomponent systems. It has the advantage that there is a large amount of eddy diffusion data available for a variety of situations. It has the disadvantage that recent work by Porter et al. (1972) and by Bell (1972) have shown that stagnant zones can exist on large trays which violate the requirement of uniform flow across the tray. On the basis of this Porter has predicted that the tray efficiency would be significantly different from that based on the eddy diffusion model for columns greater than about 3 m in diameter. However, Yanagi and Scott (1973) have recently studied columns of 1.2-m and 2.5-m diameter both with and without modified trays. The modifications to the normal cross flow arrangement were designed to produce uniform flow across the tray. They reported little difference between the efficiencies of the unmodified and the modified trays under identical distillation conditions. Therefore, since the present column is of diameter 2.13 m, and since the effect of the undoubted presence of stagnant zones is as yet uncertain, the eddy diffusion mixing model has been used in the liquid/vapor biphase. For columns greater than 3 m in diameter, the stagnant zones may reduce the tray efficiencies compared with those predicted here. A simple model has been used to provide an approximate assessment of the effect of mixing in the vapor phase, and this will be described later.

It is worth noting that slotted trays appear to give more uniform flow than normal sieve trays (Weiler et al., 1973).

THEORY

An element of the liquid/vapor biphase on a distillation tray is considered as shown in Figure 2. The element is assumed to have unit width perpendicular to the direction of liquid flow in the horizontal plane. Mixing is assumed to be complete in the vertical direction.

Equating the input and output of component i under steady state conditions, the following equation results after allowing $\delta W \to 0$ $\delta Y \to 0$ $\delta X \to 0$, etc.,

$$\frac{DeF\rho_L Q_F}{Z_l^2}\frac{d^2X_i}{dW^2} - \frac{L}{Z_l}\frac{dX_i}{dW} - \frac{X_i}{Z_l}\frac{dL}{dW} + V_{j-1}Y_{j-1\,i} - V_j Y_{ji} = 0 \quad (1)$$

Now, since W is the dimensionless tray length, and with unit width considered, and

$$Pe = LZ_l/(DeF\rho_L Q_F) \quad (2)$$

With the addition of the overall mass balance

$$\frac{dL}{dW} = Z_l(V_{j-1} - V_j) \quad (3)$$

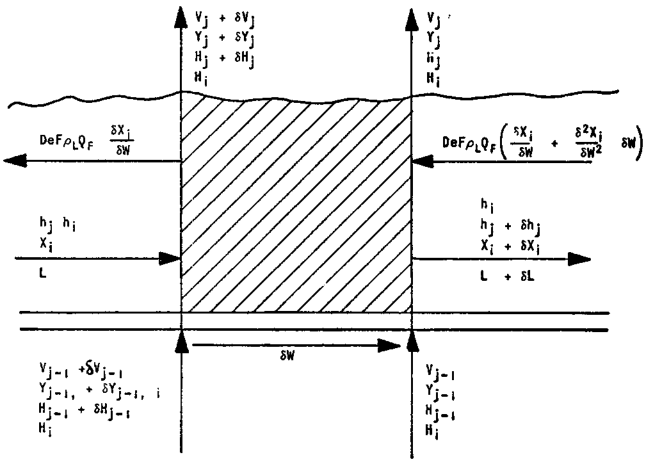

Fig. 2. Model for liquid mixing equations.

and defining a new variable

$$Z_i = \frac{dX_i}{dW} \quad (4)$$

the following equation results:

$$\frac{1}{Pe}\frac{dZ_i}{dW} = Z_i - \frac{1}{L}\left\{\frac{dL}{dW}(Y_{ji} - X_i) - V_{j-1}Z_l(Y_{ji} - Y_{j-1\,i})\right\} \quad (5)$$

An enthalpy balance yields the equation

$$Z_lV_{j-1}H_{j-1} + \frac{L}{Pe}\sum_{i=1}^{n}\frac{dZ_i}{dW}h_{ji} = \frac{dL}{dW}(h_j - H_j) + Z_lV_{j-1}H_j + L\frac{dh_j}{dW} \quad (6)$$

By substitution from Equation (5) summed for all components:

$$\frac{dL}{dW} = \frac{L\dfrac{dh_j}{dW} + V_{j-1}Z_l\left\{H_j - \sum_{i=1}^{n} h_{ji}(Y_{ji} - Y_{j-1\,i}) - H_{j-1}\right\} - L\sum_{i=1}^{n} h_{ji}Z_i}{\left\{(H_j - h_j) - \sum_{i=1}^{n} h_{ji}(Y_{ji} - X_i)\right\}} \quad (7)$$

The basic equations used by the method are Equations (4), (5), and (7).

For the particular case of no backmixing in the liquid ($Pe = \infty$), the following two equations are similarly derived:

$$\frac{dX_i}{dW} = \frac{1}{L}\left\{(Y_{ji} - X_i)\frac{dL}{dW} - V_{j-1}Z_l(Y_{ji} - Y_{j-1\,i})\right\} \quad (8)$$

and

$$\frac{dL}{dW} = \frac{V_{j-1}Z_l\left\{\sum_{i=1}^{n} h_{ji}(Y_{ji} - Y_{j-1\,i}) - H_j - H_{j-1}\right\}}{\sum_{i=1}^{n} h_{ji}(Y_{ji} - X_i) - (H_j - h_j)} \quad (9)$$

The vapor concentration above any point on the tray is obtained from the point efficiency defined in the usual way, the liquid composition and the equilibrium relationship. The local unmixed vapor flow rate is obtained from mass balance considerations. The temperature at any point is assumed to be the bubble point. Haselden and Thorogood (1964) studied the air distillation system and found that liquid and vapor temperatures were substantially at their saturation values, and so this has been used in the present simulation. In addition, Haselden and Thorogood (1964) found that the point efficiencies of the three components nitrogen, oxygen and argon were essentially equal over all the ranges of composition encountered. This will be discussed in greater detail later.

SOLUTION OF EQUATIONS

A computer program has been written to solve the equations using an ICL 1906A computer by means of a predictor/corrector method.

The tray may be thought of as being divided into N equal increments in the direction of liquid flow, and integrals are evaluated at the end points of all these increments. The problem is an initial value type, starting at the outlet weir of a tray and working across the tray against the liquid flow. At the outlet weir of any tray, the flow rate and compositions are known from the calculation of the tray below. In addition, the following boundary conditions are required:

$$\frac{dX_i}{dW} = 0 \quad i = 1, 2, \ldots\ldots$$

Starting at the outlet weir of the tray under consideration, the fourth-order Runge-Kutta method is used to obtain the integral values at the first four points. Then, Hamming's predictor/corrector method is used in a form similar to that described by Ralston and Wilf (1960). The solution continues across the tray until the inlet weir is reached. This is a stable iterative method. The result is in the form of a series of compositions of all components across the tray and flow rates at the same points.

The stability of the predictor/corrector method used is such that Peclet numbers up to 50 can be used with the tray divided into 20 intervals. Increasing the number of intervals enables higher Peclet numbers to be used.

In every case except that of plug flow in the liquid, there is a step change in composition at the inlet weir, and this is obtained by means of an overall mass balance around the entire tray after the composition profiles have been calculated. This provides the liquid starting conditions for the calculation of the next tray up.

A liquid feed is assumed to be made into a downcomer and a vapor feed is made by assuming complete vapor mixing above the feed tray. A new vapor profile is calculated. A liquid or vapor sidestream is simply taken at the average composition.

EFFICIENCY CONSIDERATIONS

At every point considered across the tray, the vapor composition above the liquid is calculated from the inlet vapor composition at that point, the liquid composition and a point efficiency defined in the usual way.

$$(E_{0G})_i = \frac{Y'_{ji} - Y'_{j-1\,i}}{Y^{*\prime}_{ji} - Y'_{j-1\,i}}$$

In a binary system the efficiencies of the two components are equal, but this is not necessarily so in a multicomponent system. A set of efficiencies must satisfy the requirement:

$$\sum_{i=1}^{n} (E_{0G})_{jiW}\, K_{jiW}\, X_{jiW} - \sum_{i=1}^{n} (E_{0G})_{jiW}\, Y_{j-1\,iW} = 0$$

Thus a set of efficiencies cannot be selected at random. In fact, in a system containing n components, only $n - 1$ may be chosen arbitrarily, and the last is fixed. This could lead to problems in the selection of the unspecified efficiency in systems with unequal efficiencies. Such inequalities have been detected (Miskin et al., 1972). However, in the present simulation, it was observed experimentally by Haselden and Thorogood (1964) that the three efficiencies were essentially equal for all compositions likely to be encountered in an upper column similar to that considered here. Thus, this removes the difficulties associated with differing point efficiencies since equal point efficiencies are acceptable.

It is not necessary to use the efficiency in the form specified above. Other efficiencies have been proposed (Holland and McMahon, 1970) and could be used in the method. However, in this simulation data is available in the conventional form from different sources, and so this form has been used.

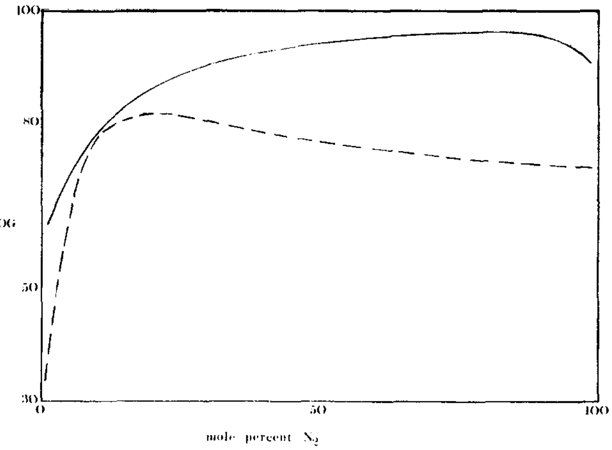

Fig. 3. Point efficiencies:—Haselden and Thorogood; ---- Brown and England.

The method allows variations in point efficiency to be taken into account. It is well established from a large amount of experimental work over many years that variations in point efficiency with composition do occur. There have been a number of explanations offered to account for these variations: (1) Variations in interfacial area (Ellis and Biddulph, 1967; Haselden and Thorogood, 1964); (2) Interfacial turbulence effects (Ellis and Biddulph, 1966); (3) Thermal effects (Liang and Smith, 1962); and (4) Variations in individual phase resistances.

In the air separation system, variations have been observed by Ellis and Catchpole (1964), Brown and England (1961), and Haselden and Thorogood (1964). The efficiencies observed by Brown and England (1961) are shown in Figure 3. These were for only the binary system nitrogen/oxygen, and a sharp reduction in efficiency was observed at low nitrogen concentration. Rather similar results were obtained by Ellis and Catchpole (1964). Foam heights of the order of 1 to 3.5 cm were observed, and these are lower than generally encountered in commercial air separation columns.

The point efficiency results of Haselden and Thorogood (1964) are also shown in Figure 3. These were for the ternary system and the line represents the approximately equal efficiencies which were found for all three components, as a function of the nitrogen composition. A column with a foam baffle at the outlet weir was used in an attempt to simulate the conditions existing at a point on a large tray. The foam heights were generally greater than those observed by Brown and England (1961).

Although these variations of point efficiency as measured in small columns have been observed by many people for many different systems, they have not been incorporated into a design program.

VAPOR MIXING

The extent of mixing which occurs in the vapor phase between the top of the froth and the next tray above has an effect on the tray efficiency of the tray above. Diener (1967) studied the magnitude of the effect and concluded that vapor mixing has a relatively minor effect on tray efficiency compared with liquid mixing. He studied the maximum possible advantage to be gained from having the liquid flow on adjacent trays in the same direction (directed flow) compared with opposite directions (normal flow). His analysis would be difficult to apply in the case

Table 1. Different Conditions Studied and Simulated for Similar Feeds and Product Streams

Run no.	Tray configuration	Point efficiencies	Mixing Liquid, pec	Mixing Vapor, V_m	Total number of trays
1	Normal	70% throughout	40	0	67
2	Normal	70% throughout	40	0.5	66
3	Normal	70% throughout	40	1.0	64
4	Directed	70% throughout	40	0	62
5	Normal	Haselden and Thorogood	40	0	60
6	Normal	Brown and England	40	0	115
7	Split	Haselden and Thorogood	10	0	66
8	Directed	Haselden and Thorogood	∞	0	57
9	Directed	Haselden and Thorogood	40	0	57

of multicomponent systems. Ashley and Haselden (1970) considered intermediate vapor mixing using a vapor cell model. Again these would not be easy to apply to multicomponent systems. Katayama and Imoto (1973) used a diffusional model for mixing in the vapor phase and concluded that this is a relatively minor effect but that it is not necessarily negligible in large columns.

In commercial air separation columns, which have very small tray spacing, perhaps as little as 10 cm, it is almost certain that very little lateral mixing takes place in the very small distance between the top of the froth and the tray above. Therefore, an adequate simulation can probably be achieved by assuming no mixing in the vapor phase. However, for the sake of completeness, it was felt that it should be possible to evaluate the effect of vapor mixing in this type of column. A diffusional model would have increased the computation time significantly, and so, a very simple vapor mixing model was used, as follows.

A vapor mixing number V_m is defined so that if there is no mixing in the vapor phase, $V_m = 0$. In this case the vapor compositions and flow from any point on the tray are not changed at all before they are used at a corresponding point, as the inlet vapor to the tray above. If the vapor mixing is assumed to be complete, then $V_m = 1$. In this case, the vapor flows and compositions at all points are equalized out to the average values. Thus the inlet vapor to the tray above has constant composition and flow rate at all points on the tray. This is assumed to be the case for the reboiler vapor approaching tray 2.

For intermediate vapor mixing between trays, V_m is between 0 and 1 and its significance is as follows. The vapor composition profile across the tray is assumed to become linear rather than the slightly curved unmixed profile. Furthermore, the approach of the new vapor concentration above the outlet weir to the completely mixed profile is equal to V_m. Thus, a new composition profile for each component is calculated such that the approach to the completely mixed value above the outlet weir is equal to V_m, and the average value of composition occurs at the center point of the tray. Also, the flow rate of vapor at all points on the tray is assumed to equalize out in the cases of intermediate and complete mixing.

This is a very simplified model, but it is felt to be adequate to allow the relatively minor effect of intermediate vapor mixing to be taken into account. The closer intermediate mixing comes to complete mixing, the better will this model be.

COLUMN SIMULATION

Nine different conditions were studied and simulated for similar feeds and product streams. The main feed to the column was put in to be just below the pinch point which develops in this part of the column, a similar composition location being used in all cases. The argon offtake was made when the argon concentration had almost reached the peak which occurs in this section. The argon return was put in one tray below. The variables studied were the effect of directed flow compared with normal flow, intermediate liquid mixing compared with plug flow, the effect of using constant point efficiencies of 70% for each component and using Haselden and Thorogood (1964) measured efficiencies or the Brown and England (1961) efficiencies, the effect of vapor mixing varying from complete through intermediate to no mixing, and the effect of split flow trays compared with single crossflow trays. The conditions are summarized in Table 1.

The Peclet number of 40 was calculated from mixing studies carried out in an air/water simulator with small hole size trays, (Biddulph, 1975). The equilibrium data used was from A.F. Aero Propulsion Laboratory (1964). The equilibrium constant (K value) data were fitted by quadratic equations using the reciprocal of the absolute temperature based on conditions existing at points in the top, middle, and bottom of the column. Thus, the composition effect on K values was included. A check was made to ensure that no maxima or minima had occurred within the temperature range of interest. The liquid and vapor enthalpy data were fitted by quadratic equations in absolute temperature, and a similar check made.

Run 5 incorporates the conditions which are probably closest to an actual operating column. The conditions predicted by this solution are shown in Tables 2 and 3.* Table 2 shows the compositions of liquid and vapor on trays 2 to 60. The reboiler is considered to be tray 1. The data input for the program is given in Table 5.

Figure 4 shows the results plotted in a similar form to that used by Latimer (1967). This shows a very similar profile to the theoretical tray profile given by Latimer (1967), and this is encouraging since Latimer (1967) reports that a tray efficiency of about 100% is reasonable based on plant experience. Thus, the 60 trays required in this simulation compares well with the 63 theoretical trays

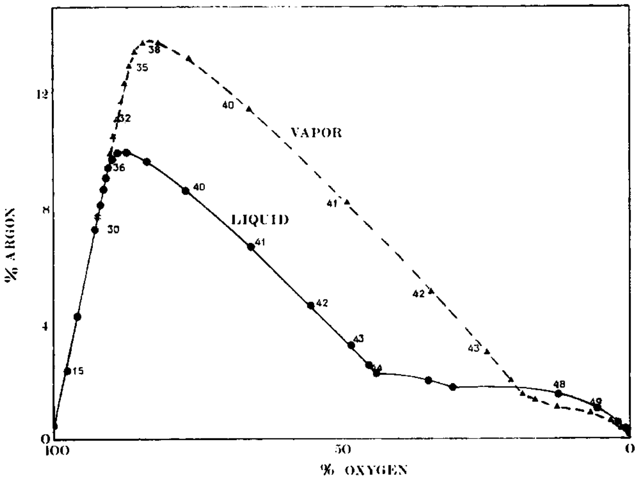

Fig. 4. Composition profile.

* Tables 2, 3, and 5 have been deposited as Document No. 02562 with the National Auxiliary Publications Service (NAPS), c/o Microfiche Publications, 305 E. 46 St., New York, N. Y. 10017 and may be obtained for $3.50 for microfiche or $11.30 for photocopies.

predicted by Latimer. The recent work by Ashley and Haselden (1972) has indicated that there may be a slight reduction in point efficiencies due to the presence of vapor voids, but this is felt unlikely to be significant on these trays.

Table 3 shows the other conditions in simulation run 5, the flows, temperatures, and efficiencies. The point efficiency used on a given tray was predicted from the data of Haselden and Thorogood (1964) when the solution was commenced at the outlet weir. The same point efficiency was used for each component as discussed earlier. The units of liquid flow are lb. mole/s ft., and the units of vapor flow are lb. mole/s (ft^2). Temperature readings are in °K.

The temperature profile through the column is shown in Figure 5.

The Murphree plate efficiencies were calculated for each component on every tray, and these are shown in Table 3. These are plotted in Figure 6. It can be seen that wide variations in plate efficiency occur through the column. Very high or very low apparent efficiencies occur near feed locations and around the peak in the argon concentration. At the bottom of the column, the oxygen and argon efficiencies are the same, while the nitrogen efficiency is much higher. This is to be expected from the effect of the equilibrium relationship. At the top of the column the oxygen efficiency is slightly the lower, with the nitrogen efficiency tending towards the argon efficiency.

This illustrates the fact that in multicomponent systems a tower cannot be accurately designed by using a simple ratio of plate efficiency to point efficiency for all components. The characteristics of multicomponent systems must be allowed for. It has often been stated that the severe falls in efficiency which have been observed in small columns have not been found in larger commercial columns. From the results here it can be seen that this is to be expected from the effect of lack of mixing on the larger trays.

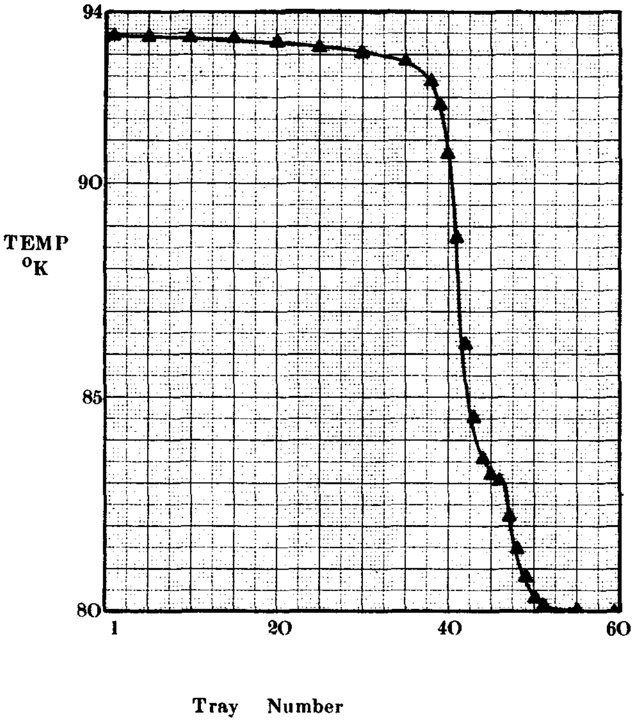

Fig. 5. Temperature profile in simulation run 5.

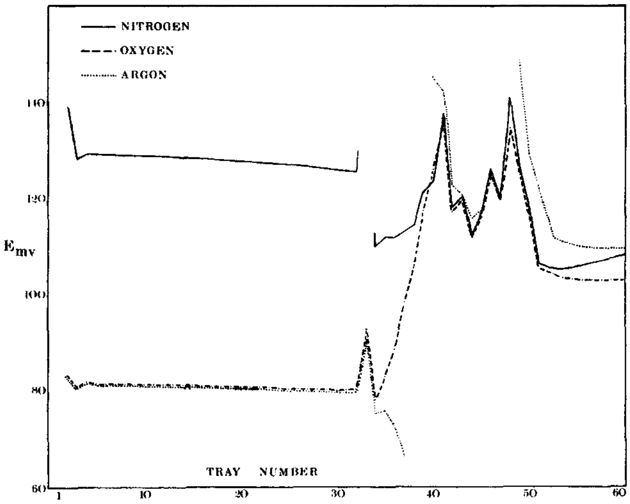

Fig. 6. Murphree tray efficiencies in simulation run 5.

COMPARISON OF COLUMNS

It has been mentioned that nine different simulations were made, representing different conditions possible in the column. The conditions have been shown in Table 1. Simulation number 5 has been discussed in some detail, and now the important points arising from the other runs will be discussed. All the runs were made with the same conditions of sidestreams and feeds.

EFFECT OF VAPOR MIXING

The extent of mixing occurring in the vapor space between trays is known to be a relatively minor one, and with the very small tray spacing typical of air separation columns the vapor is very unlikely to mix significantly. Nevertheless, three runs were made with the object of assessing the possible effect. Runs 1, 2, and 3 were made with point efficiencies constant at 70% throughout the column. In run 1, no vapor mixing was included. In run 3, complete mixing was used in the vapor ($V_m = 1$). In run 2, intermediate mixing was used with $V_m = 0.5$. It con be seen that with complete mixing in the vapor, the column required 64 trays while with no mixing the column required 67 trays. Intermediate mixing led to a column with 66 trays.

EFFECT OF DIRECTED FLOW

It has been known for many years that, unless the vapor phase is completely mixed, there is an advantage in terms of tray efficiency in directed flow as compared with normal flow. This comparative performance has been studied with runs 5 and 9 and runs 1 and 4.

In runs 5 and 9, the experimental point efficiencies of Haselden and Thorogood (1964) were used, with no vapor mixing, and it can be seen from Table 1 that the directed flow column had 3 fewer trays for the same performance. Latimer (1967) observed that directed flow is only of significant advantage with values of point efficiency greater than 60%. In this column simulation, more than half the trays are operating at a point efficiency of about 60%. Thus only a marginal improvement is to be expected.

The directed flow tray efficiency has been compared with the normal flow tray efficiency in the lower and upper sections of these columns. In the lower section the percentage improvements for the three components were: nitrogen, 17%, oxygen, 6.4% and argon 6.4%. In the upper section, the improvements were nitrogen 18%, oxygen 12%, and argon 17%. Thus the advantage of directed

TABLE 4. SIMULATION RUN 1

Tray	E_{OG}	$E_{MV}N$	$E_{MV}0$	$E_{MV}A$
41	70.000	82.3781	82.2783	82.8173
40	70.000	80.7570	80.3034	82.7835
39	70.000	85.0068	84.8521	85.7271
38	70.000	84.9584	84.3980	87.6563
37	70.000	94.2945	93.9505	96.0720

flow is different for the different components, as would be expected. This fact makes the use of a simple ratio of efficiencies to assess the relative advantages of directed flow for multicomponent systems suspect.

A similar comparison of normal and directed flow was made using constant point efficiencies of 70% throughout the column in runs 1 and 4. Again no mixing was assumed in the vapor phase. This comparison showed an improvement of 5 trays for the directed flow column. This slightly extra improvement is expected due to the higher point efficiencies in the bottom section of the column.

ALTERNATIVE POINT EFFICIENCIES

The point efficiencies determined by Brown and England (1961) are shown in Figure 3. It can be seen that a very severe decrease was observed at low nitrogen concentrations. These were used in simulation run 6 by assuming that all three components exhibited equal point efficiencies. This simulation resulted in a column containing 115 trays. This is many more trays than is typically used, and so this indicates that efficiency falls as severe as this are probably not experienced in commercial columns. This is probably due to the fact that the conditions in the column used were not representative of the conditions at a point on an operating large-scale tray. The column used by Brown and England did not have a foam baffle, whereas the column of Haselden and Thorogood (1964) did have such a baffle. This may indicate that a foam baffle is desirable in small column studies to assist in producing representative point efficiencies.

EFFECT OF SPLIT FLOW

The definition of the Peclet number leads to the fact that in a split flow column, for equal values of eddy diffusivity, foam density, etc., the Peclet number is divided by 4. Thus, in studying the split flow column (Run 7), half the column was simulated using a Peclet number of 10. Again, the point efficiency values of Haselden and Thorogood were used, with no vapor mixing. A column having 66 trays was the result. This suggests that 6 extra trays would be required to achieve the same duty. This is assuming that the eddy diffusion model applies. In reality, it may well be that the difference is not as great as this. The recent work of Lim et al. (1974) has indicated that because the effect of any stagnant zones which are present will not be as severe for split flow columns, the disadvantage in this diameter column would be reduced. They predict that there would even be an incentive to go to split flow in very large columns.

PLUG FLOW IN THE LIQUID

In order to check the magnitude of any possible further reduction in column size, a run was made (run 8) with plug flow in the liquid rather than the Peclet number of 40. Although this did lead to slightly higher efficiencies in parts of the column, in fact the number of trays came out to be the same, at 57, compared with run 9.

OSCILLATING EFFICIENCIES

A minor effect which has been observed is the fact that in the normal flow configuration, the efficiencies can go up and down on adjacent trays. This has also been noted by Lockett et al. (1973). This can be seen in some results taken from the middle region of run 1, and shown in Table 4. The oscillating effect in nitrogen efficiencies superimposed on a general downward trend in efficiency is shown in Figure 7. This is due to alternate flattening of the vapor concentration profile on successive trays due to the way in which the liquid and vapor profiles combine. This is illustrated in Figure 8. The effective vapor composition slope across the tray is represented by the composition of nitrogen above the inlet weir (V'') minus the composition of nitrogen above the outlet weir (V'). The vapor composition profile between trays is alternately more and less advantageous. This effect is a minor one, and it is completely absent in directed flow, as would be expected.

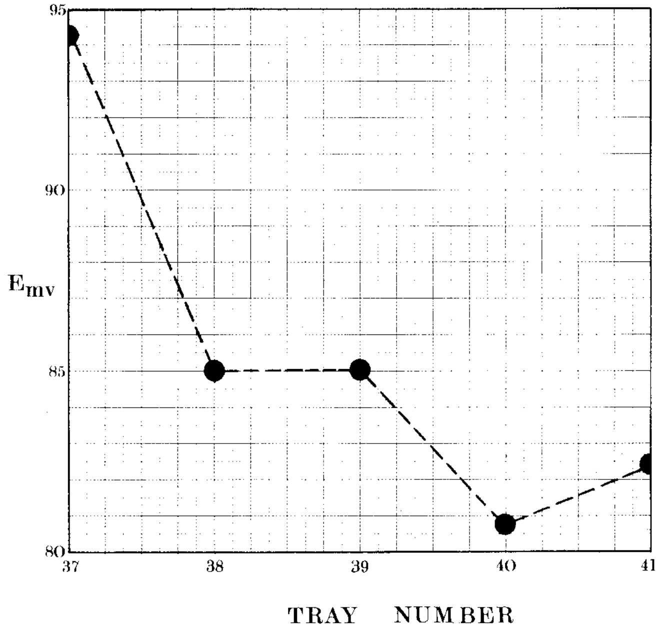

Fig. 7. Oscillating nitrogen tray efficiencies in simulation run 1.

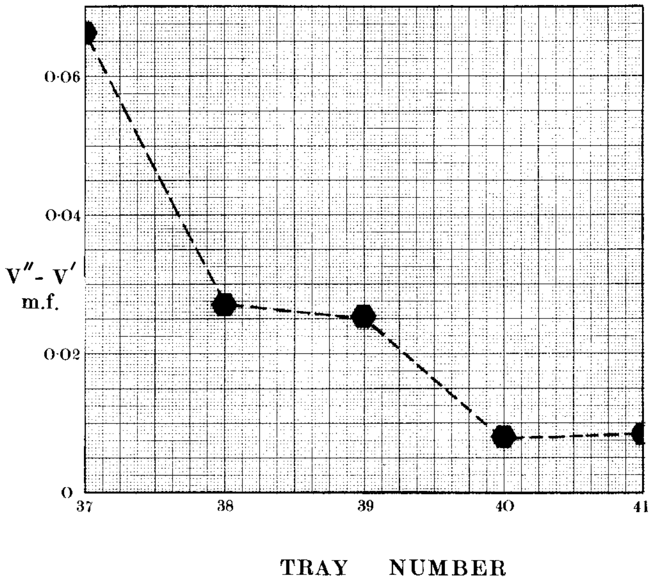

Fig. 8. Effective vapor concentration profile slopes for nitrogen, run 1.

CONCLUSIONS

This paper has illustrated the use of a model based on mixing characteristics and point efficiencies to simulate commercial-scale columns. Apart from any direct interest in the air separation column under consideration, some general points about columns distilling multicomponent mixtures are brought out.

It is true that the system studied here does have a simplifying property which is not necessarily shared by other multicomponent systems; that is, it has been shown experimentally that all three components exhibit the same point efficiency at any given composition. In general, the different components would exhibit different point efficiencies. Nevertheless, the study has indicated some effects which would be difficult to assess from binary studies, namely the effect of various column configurations on different components.

Other columns operating with other systems would naturally behave differently. The mixing characteristics on other trays would probably be different from those of the small hole size sieve trays used in air separation columns. Vapor and liquid loadings would be different as well as tray spacing. The behavior of other systems in other columns is currently under investigation where detailed column data are available.

The simulation of the present column has brought out some interesting points. The benefit of directed flow compared with normal flow has been assessed for this particular column. It has been shown that directed flow benefits different components by differing amounts, as would be expected. The simulation using the measured point efficiencies of Haselden and Thorogood (1964) gives good agreement with plant experience. The severe point efficiency decreases reported by Brown and England (1961) do not appear to be experienced on large-scale columns. This leads to the conclusion that the use of foam baffles may be desirable in small-scale columns in order to give representative point efficiencies. A minor effect of oscillating efficiencies on successive trays in the normal flow regime is not present in directed flow.

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NOTATION

A = cross-sectional area of froth, L^2
De = eddy diffusion coefficient, L^2/T
E_{mv} = Murphree plate efficiency, based on vapor phase
E_{OG} = point efficiency based on vapor phase
F = froth height, L
h = liquid enthalpy, molal
H = vapor enthalpy, molal
K = equilibrium const. (Y^*/X)
L = liquid flow rate, kg moles/T/unit width
n = number of components
Pe = Peclet number $= Z_l L/(De\, F\, \rho_L\, Q_F)$
Q_F = relative froth density, m^3 liquid /m^3 froth
T = temperature, °K
V = vapor flow rate, kg moles/T/unit area
V' = vapor composition above outlet weir, mole fraction
V'' = vapor composition above inlet weir, mole fraction
W = dimensionless flow path length
X = mole fraction in liquid
Z_l = liquid path length, L
Y = mole fraction in vapor
ρ_L = liquid density, molal

Subscripts

i = component i
j = Tray j
$j-1$ = Tray $j-1$ (numbering upwards)
w = at Point w on a tray
$*$ = equilibrium value
$'$ = at point on the tray
1, 2, . . . = component 1, 2, . . .
N = nitrogen
O = oxygen
A = argon

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Freeze Dehydration by Microwave Energy:

Part I. Theoretical Investigation

A general unsteady state analysis is employed to derive a mathematical model of a freeze-drying process using microwave heating. The model takes into account the variations of the transport and dielectric properties in the sample with both time and location as a function of temperature and pressure. The variations of the properties are described by functionals which have been derived from literature data and are built into the model.

The mathematical model is used to simulate the freeze drying of beef meat with microwave energy at 2450 MHz. The simulation shows that drying rates are essentially a function of the microwave power input. The model also shows that the total pressure and the partial pressure of water vapor in the vacuum chamber directly affect the sample temperature during dehydration. The simulation shows, in particular, that, an optimal microwave freeze-drying operation corresponds to an operation near corona and overheating/melting conditions.

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SCOPE

Microwave dielectric heating has shown a great potential in accelerating freeze drying (Jackson et al., 1957; Copson, 1958). A reduction of drying time by factors of 3 to 13 has been reported when conventional (radiant) heating is replaced by microwave dielectric heating (Hoover et al., 1966). A continuous or semicontinuous process may thus be employed. Dissipation of microwave energy throughout the bulk of the material, particularly in the frozen core, accounts for the reduction of the drying time as the problem of supplying the enthalpy of sublimation by conduction from the surface is overcome.

However the lack of a systematic theoretical study of the microwave freeze drying process, as well as problems arising from applying the relatively new microwave heating technology, seem to have hampered the development of this new technique. The present work is intended to provide a mathematical simulation of the freeze drying process using microwave dielectric heating. Assuming an infinitely sharp sublimation front which retreats uniformly, a one-dimensional model is developed and used to simulate the freeze drying of beef meat with microwave energy at 2450 MHz. Effects of the microwave power input, the total pressure, and the water vapor pressure of the system and the sample thickness upon the drying process are investigated. Such a parametric study is essential for a better understanding of the freeze drying process and provides a useful tool for future process design, optimization and control.

CONCLUSIONS AND SIGNIFICANCE

Application of the mathematical model to the freeze-dehydration of beef meat at 2450 MHz shows that drying rates are essentially a function of the microwave power input. The total pressure and the partial pressure of water vapor in the vacuum directly affect the sample temperature during drying but have little effect on the drying time. Low operating vacuum chamber pressures are necessary to ensure a temperature of the frozen core as low as possible and thus allow one to use a higher microwave power input to shorten the drying time. However, pres-

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