

Validating

THE EQUILIBRIUM STAGE MODEL

for an Azeotropic System in a Laboratorial Distillation Column

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During their fourth year of undergraduate studies, chemical engineering students at the Instituto Superior de Engenharia de Coimbra (ISEC), Portugal, take a full laboratory course in unit operations and process control. The topics covered include evaporation, distillation, absorption in packed columns, solid-liquid extraction, drying, and the control of variables often found in industrial units (*e.g.*, pressure, flow, level, and temperature) employing laboratory units or bench-scale kits. The course's basic aim is the practical demonstration of theoretical concepts taught in courses on process separation, chemical thermodynamics, and process dynamics at laboratory scale. It also provides students with experience in operating and controlling complex units. Regarding the work on distillation, the students are asked to validate the steady-state behavior of a laboratory unit used for separating an azeotropic mixture of aniline and water. The interest in this binary system arose from an intensive research program carried out in the chemical engineering department of ISEC in collaboration with a Portuguese company that produces aniline—with the aim of optimizing the aniline production section. In addition, this work also aims to validate knowledge relating to the distillation of heterogeneous azeotropic mixtures, of which the aniline-water system is a simple and easily handled example.

The conceptual basis used to describe the phenomena involved in a distillation column is the equilibrium stage model, which assumes thermodynamic equilibrium between

the species and perfect mixing in each phase and tray.^[1, 2] But it is quite common for equilibrium not to be achieved in vapor-liquid-liquid dispersions arising from heterogeneous azeotropic mixtures. This is because of the occurrence of kinetically controlled phenomena, such as mass transfer, coalescence, and nucleation in liquid phases. Regardless of

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the mismatch of theoretical assumptions and real behavior, the equilibrium stage model is still used to represent the operation of distillation columns phenomenologically, and several research groups have presented data for three-phase distillation experiments to validate it.^[3-6] Thus, this work aims simultaneously to enable students to gain experience in operating and analyzing a distillation procedure, to use vapor-liquid equilibrium (VLE) prediction methods, and to contribute to the research community's efforts to validate the equilibrium stage model for the aniline-water system.

Three four-hour sessions are required to complete the work. The first is devoted to a review of the basic theory behind mixture thermodynamics and methods for predicting activity coefficients for VLE, analysis of the column layout, and understanding its operation and control. Between the first and second sessions, the students develop an Excel workbook to obtain the VLE prediction for the aniline-water system at atmospheric pressure. Each group of three or four students is asked to use a different prediction method for the activity coefficients among UNIFAC, UNIQUAC, two-constant Margules, and van Laar,^[7] then to compare the results with experimental data published in the literature for the aniline-water system at atmospheric pressure.^[8, Appendix G] During the second session, the students carry out the experimental work with the distillation column, running it until steady-state conditions are reached. Next, they use Aspen Plus v. 11.1 to compute the unit steady state with an equilibrium stage-model-based module. Finally, in the third session, the results are presented, compared with those given by simulation, and discussed.

EXPERIMENTAL EQUIPMENT AND SAMPLING

Aniline, even in low concentrations, is a fairly toxic aromatic hydrocarbon. Its handling therefore requires students take some safety precautions, that is, to wear protective clothing, gloves, and eye/face protection to avoid skin contact. Furthermore, the work is carried out in a well-ventilated area to reduce the toxicity risk.

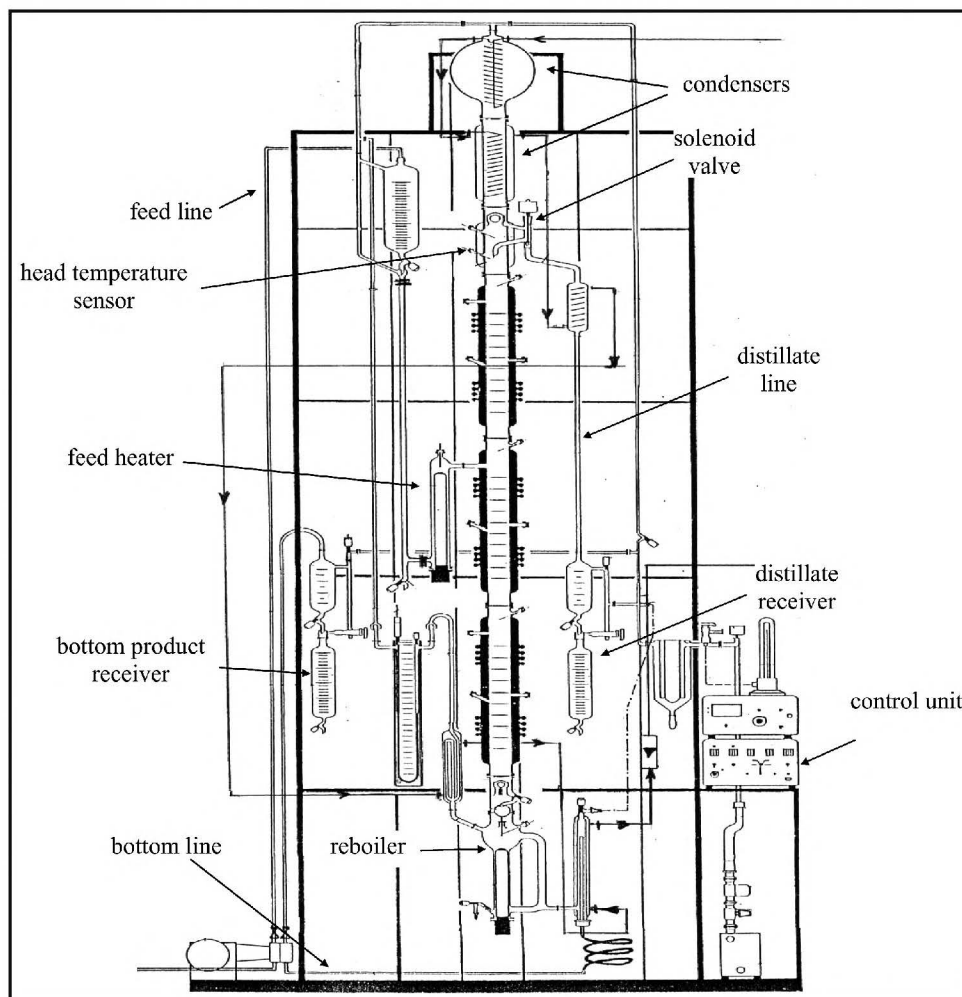
Figure 1. Schematic diagram of laboratory unit used for experiments.

The schematic diagram of the column where experiments are performed is shown in Figure 1. The unit is formed by three column sections, each with 10 bubble-cap trays, a total condenser, and a kettle-type reboiler (reference Labodest 250 from Fischer). The column body is made of glass with an internal diameter of about 0.05 m.

The feed stream enters in tray 11, and the reboiler, which is the last tray of the column, operates simultaneously as a heat exchanger and equilibrium tray, since it contains an electrical-resistance element with maximum heating capacity of 3 kW.

The schematic representation of trays is shown in Figure 2. The net area for vapor flow (6) is 10% of the total area of the tray. Two cavities for liquid inlet (1) and outlet (2), with slightly different heights, separated by a wall (3), form the bubble caps. The liquid falls from the upper tray into the reflux zone (4) through the downcomer, circulates around the wall to the opposite position, and is discharged to the lower tray through the tube (5). This design increases the contact time between the vapor and liquid phases.

A solenoid valve controls the reflux flow to the column



(Figure 1). When the valve is open, a glass stem is pulled magnetically from the seat and the liquid from the condenser is collected in the distillate receiver. When the valve is closed, the stem is pushed back, the seat is closed, and, when it is partially filled, the liquid overflows through a side tube and returns to the column (Figure 3). The reflux ratio value is set by employing two time preselectors on the control device, thus establishing the valve dead band. For the aniline-water binary system, however, the control of the distillation column based on the reflux ratio causes severe problems due to the forma-

tion of two immiscible liquid phases in the condenser—the organic being denser than the aqueous at the temperature at which it leaves the condenser. The difference in density means that, when the valve opens after being closed for a while, a small volume of liquid retained in the valve seat (below the side tube level) is poured into the distillate receiver. This produces significant changes in the distillate composition since it is rich in the heavier phase (the organic phase). Table 1 indicates the density values for the aqueous and organic phases formed at different temperatures for the aniline-water system.^[8, Appendix G]

temperature (°C)	density (kg/m ³)	
	aqueous phase	organic phase
20	999	1023
30	997	1014
40	995	1006
50	991	998
60	987	989
70	982	982

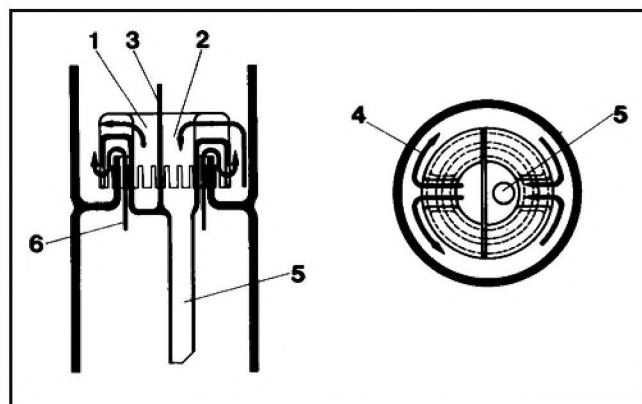


Figure 2. Schematic representation of column trays.
1. Cavity for liquid inlet. 2. Cavity for liquid outlet.
3. Wall. 4. Reflux zone. 5. Downcomer to the lower tray.
6. Vapor flow trajectory.

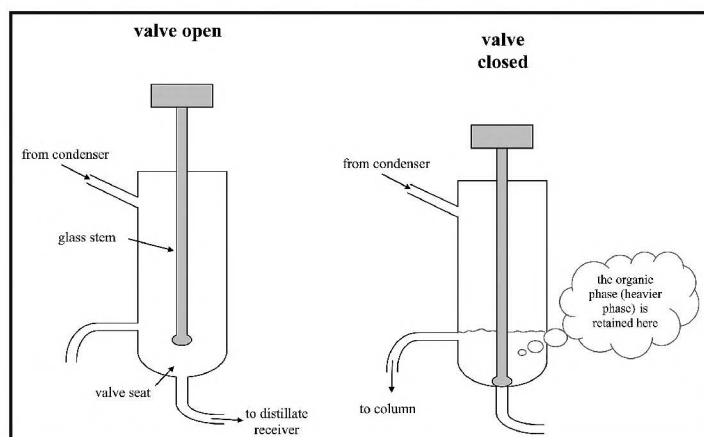


Figure 3. Schematic detail of the solenoid valve operation: open and closed positions.

To overcome this drawback, instead of reflux ratio adjustment, an on-off control scheme based on the boiling point limit in the upper tray of the column is employed, with the head temperature measured through a resistance thermometer (Figure 1). Whenever it exceeds the value selected at the control unit (98.7 °C—the azeotropic temperature), the distillate flow rate is automatically interrupted, and the condensate starts to flow back to the column. Consequently, the temperature of the upper tray starts to fall, and when it reaches the preselected value the distillate starts to be collected again. This control scheme leads to small changes in the position of the solenoid valve, which is open most of the time.

The feed stream is preheated to 99.3 °C before entering the column in liquid state at atmospheric pressure. The feed stream is sampled for the quantitative determination of aniline concentration in the mixture.

When the steady state is reached, the students collect the distillate and bottom products in graduated receivers for a period of 90 minutes. At the end, the distillate is transferred to a separatory funnel, and after the separation of the two phases, the volume of each layer is measured in graduated cylinders.

The aniline concentrations in the aqueous phase of distillate, in the bottom product, and in the feed sample are quantitatively determined by spectrophotometry, after appropriate dilution. The absorbance of the solutions is measured at 279.5 nm in a UV-Vis spectrophotometer unit after setting the calibration line. The quantitative analysis of water concentration in the organic phase of the distillate is determined by titration with Karl Fisher reagent.

For the range of flows used in the experiments, the column manufacturer indicates that the Murphree efficiency is 92%. The experimental confirmation of this value is not performed exactly because of the column configuration, which does not allow the extraction of liquid samples in consecutive trays.

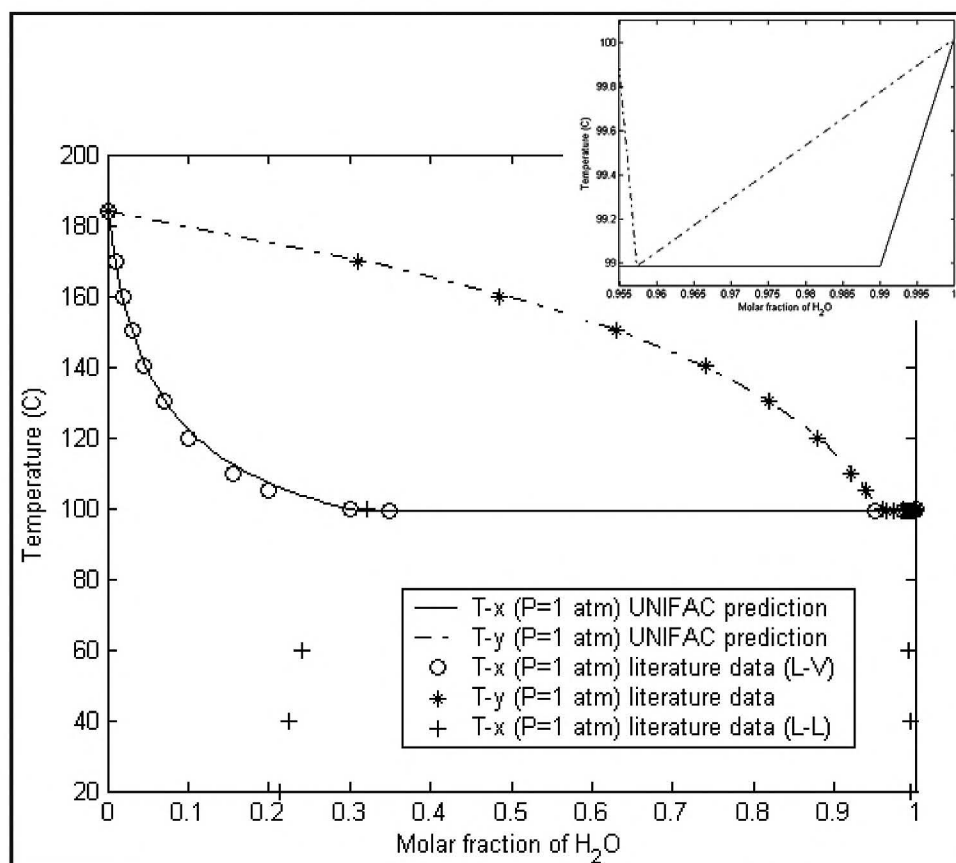
MODEL VALIDATION

Aspen Plus v. 11.1 is used to validate the equilibrium stage model; the steady-state flows, compositions, and temperatures of the upper tray and bottom stream result-

ing from the model solution are compared with laboratory data. The Radfrac module is chosen to describe the column unit since it is based on the rigorous solution of the equilibrium stage model for multistage vapor-liquid fractionation, steady-state operations.^{9, 10} The model consists of a set of nonlinear algebraic equations, comprising the material balance (M) and thermodynamic equilibrium relation (E) for each component and tray, and the summation of mole fractions (S) and enthalpy balance (H) for each tray, generally called MESH equations.¹¹

This system can be augmented with the trays' hydraulic relations and pressure-drop profiles across the column when the unit geometry is known. The broader generality of the Newton-Raphson algorithm led this to be chosen to solve Radfrac module in rating mode. The Newton-Raphson algorithm implemented is based on the classic Naphtali and Sandholm algorithm.¹² First, the number of equations and variables resulting from unit modeling is reduced through the condensation of mole fractions, liquid, and vapor flows into new variables representing component molar flows. Next, the complete set of variables is ordered, and the resulting algebraic equation system solved iteratively by employing a Newton-type algorithm. The convergence is checked after each iteration by comparing the sum of squares of all variables, conveniently weighted by scale factors, with a tolerance defined as a function of the number of degrees of freedom the system involves and inlet flows. An azeotropic convergence algorithm is chosen to handle the current binary system that forms a minimum-boiling azeotrope in the region of low aniline concentrations. The operating conditions, including the molar flow of distillate stream, the heat consumed in reboiler, the stages at which streams enter/leave the unit, the pressure-drop profile across the column, additional information regarding the condenser operation, and the characterization of the second liquid phase—formed essentially by aniline—are introduced into Aspen Plus. Molar flows are set equal to the experimental steady-state values, and the pressure drop is

Figure 4. Comparison of experimental data from literature^[8, Appendix G] vs. VLE data determined through UNIFAC for aniline-water system.



disregarded due to the small flows involved in the operation. The characteristics of the feed stream, including its temperature, pressure, and molar composition, are also entered into Aspen Plus. It is considered that there is no sub-cooling in the condenser and the Murphree stage efficiency is set to 92%. The Appendix at the end of this paper presents the Aspen Plus Input Summary file for a successfully converged model.

RESULTS

The first step in analyzing the results is to compare the VLE data calculated by the Aspen Properties module with the prediction obtained by students. Next, both must be validated with experimental data. The diagram in Figure 4 shows the agreement between the VLE data predicted using the UNIFAC method and the experimental data published in the literature.^[8, Appendix G] The system presents a heterogeneous azeotrope at 98.7 °C and 0.044 of aniline mole fraction, where three phases are in equilibrium: a vapor phase and two liquid phases [an organic phase with 30.3% (mole/mole) water, and an aqueous phase with 98.6% water].

This happens because the vapor-liquid envelope overlaps the liquid-liquid envelope, as illustrated in Figure 4. This task allows students to understand that for heterogeneous azeotropes the vapor formed during boiling has the same composition as the overall liquid, but the three phases in equilibrium have distinct compositions, contrary to what

happens for homogeneous azeotropes, where the liquid and vapor formed have the same composition.

The VLE prediction methods using UNIQUAC, two-constant Margules, and van Laar activity-coefficient models require binary parameters for the aniline-water system, which students estimate by employing the following procedure and theoretical basis.

For a binary system containing two liquid phases and one vapor phase in equilibrium, the fugacities of each compound in each of the phases are equal. That is:

$$\underbrace{\gamma_{as}^{\text{org}} P_a^* X_{as}^{\text{org}}}_{\text{fugacity of aniline (a) in the organic phase}} = \underbrace{\gamma_{as}^{\text{aq}} P_a^* X_{as}^{\text{aq}}}_{\text{fugacity of aniline (a) in the aqueous phase}} = \underbrace{P y_a}_{\text{fugacity of aniline (a) in the vapor phase}} \quad (1)$$

and

$$\underbrace{\gamma_{ws}^{\text{org}} P_w^* X_{ws}^{\text{org}}}_{\text{fugacity of water (w) in the organic phase}} = \underbrace{\gamma_{ws}^{\text{aq}} P_w^* X_{ws}^{\text{aq}}}_{\text{fugacity of water (w) in the aqueous phase}} = \underbrace{P y_w}_{\text{fugacity of water (w) in the vapor phase}} \quad (2)$$

when the vapor phase behaves like an ideal gas mixture. The expressions γ_i^{org} and γ_i^{aq} represent the activity coefficients of component *i* in the organic and aqueous phases, respectively; X_i^{org} and X_i^{aq} are the molar fractions of component *i* in the organic phase and aqueous phases, respectively; P_i^* is the

vapor pressure of the pure component *i* at temperature *T*; *P* is the pressure; and y_i is the mole fraction of component *i* in the vapor phase. The subscript *s* stands for saturated liquid phases.

According to the phase rule, a binary system with three phases in equilibrium has just one degree of freedom, which means that by fixing the pressure (atmospheric pressure) the system becomes determined. Setting the activity coefficient model, the functional forms of γ_a and γ_w can be explicitly written, and the preceding equations lead to

$$\gamma_{as}^{\text{org}} (A_{a,w}, A_{w,a}, X_{as}^{\text{org}}) X_{as}^{\text{org}} = \gamma_{as}^{\text{aq}} (A_{a,w}, A_{w,a}, X_{as}^{\text{aq}}) X_{as}^{\text{aq}} \quad (3)$$

and

$$\gamma_{ws}^{\text{org}} (A_{a,w}, A_{w,a}, X_{ws}^{\text{org}}) X_{ws}^{\text{org}} = \gamma_{ws}^{\text{aq}} (A_{a,w}, A_{w,a}, X_{ws}^{\text{aq}}) X_{ws}^{\text{aq}} \quad (4)$$

where $A_{a,w}$ and $A_{w,a}$ are the binary interaction parameters of the model chosen for the aniline-water system. When the liquid-liquid equilibrium data is available, the fractions X_{as}^{org} , X_{as}^{aq} , X_{ws}^{org} , and X_{ws}^{aq} can be used to evaluate the two parameters $A_{a,w}$ and $A_{w,a}$. Solubility data of aniline in water and of water in aniline for a temperature range of 20 °C to 100 °C can be found in the reference,^[8, Appendix G] thus allowing students to estimate mutual solubility values at the azeotrope temperature (98.7 °C). The parameters obtained are used to calculate activity coefficients for subsequent vapor-liquid equilibrium calculations in the regions of $0 < x_w < X_{ws}^{\text{org}}$, and $X_{ws}^{\text{aq}} < x_w < 1$. Table 2 lists the parameters obtained by the students for the UNIQUAC, two-constant Margules, and van Laar activity coefficient models.

The results of the Radfrac module are compared with experimental results in Table 3, showing the agreement

TABLE 2 Values of Binary Interaction Parameters for UNIQUAC, Two Constant Margules, and van Laar VLE Prediction Models		
model	binary interaction parameters	
	$A_{a,w}$ (J mol ⁻¹)	$A_{w,a}$ (J mol ⁻¹)
UNIQUAC	1524	575
two-constant Margules	6247	5836
van Laar	13164	4798

TABLE 3 Comparison of Experimental Data with Model Predictions	
Operating Conditions	
Feed: Flow: 2.623 l/h = 2.619 kg/h Molar flow: 132.22 mol/h (100% liquid) Temperature: 99.3 °C Pressure: 1 atm Aniline mole fraction: 4.53×10^{-3}	Distillate: Molar flow: 17.72 mol/h Reboiler: Heat duty: 335 W
Laboratory data	RadFrac results
Distillate: Temperature: 98.7 °C Aniline mole fraction: 0.0353	Distillate: Temperature: 98.98 °C Aniline mole fraction: 0.0338 Reflux ratio: 0.645
Bottom product: Molar flow: 114.63 mol/h Temperature: 101 °C Aniline mole fraction: 1.14×10^{-6}	Bottom product: Molar flow: 114.50 mol/h Temperature: 100.02 °C Aniline mole fraction: 1.16×10^{-6}

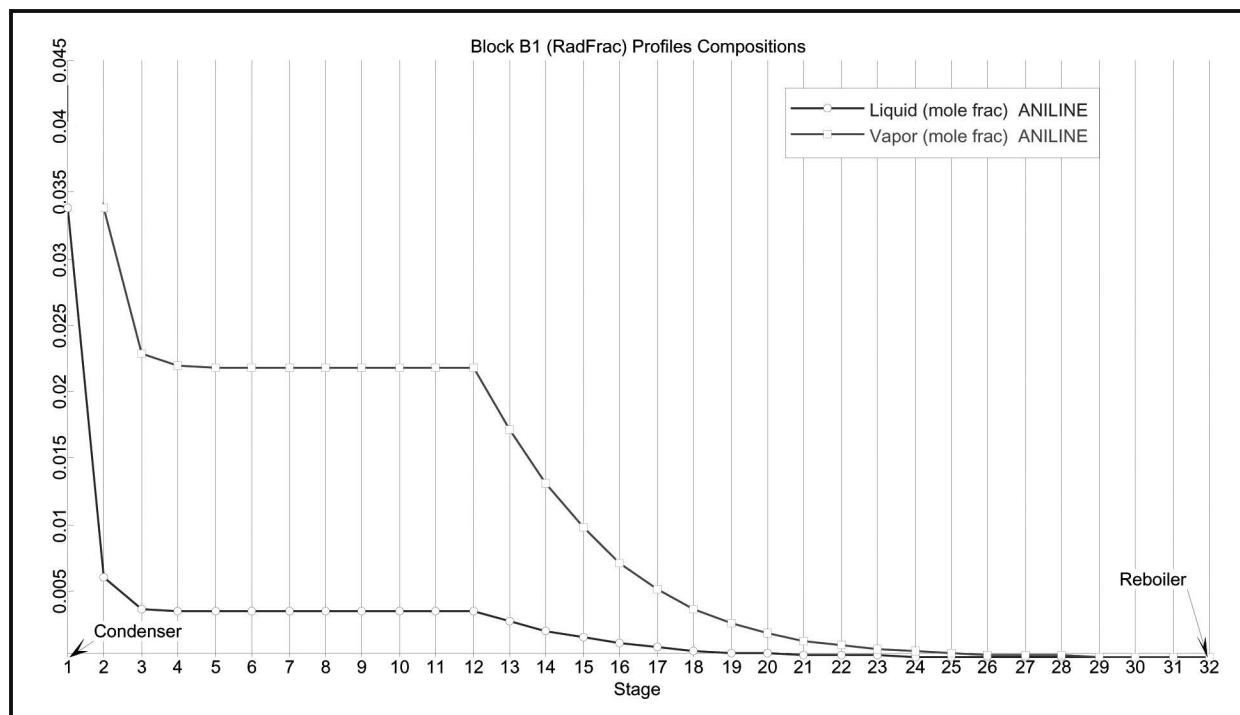


Figure 5. Composition profiles of aniline across the column.

between the model's prediction and experimental data, thus validating the equilibrium stage model for the aniline-water system. Once the heat duty in the reboiler is introduced into the model, in rating mode, it is able to determine the reflux ratio, which just represents an average value since, with the control strategy implemented, it varies discretely between 0 and ∞ , depending on the valve position. Indeed, such a value represents a possible set-point value, if the control scheme was based on the reflux ratio.

Using the Profiles form, it is possible to view the results from Radfrac as compositions, temperatures, and flow rates for each column tray. Figure 5 shows the profiles of aniline composition in both liquid and vapor phases across the column. As expected, the aniline concentration in both liquid and vapor streams increases from the bottom to the top of the column, with the aniline mole fraction in the vapor always being greater than that in the liquid since the feed stream is located to the right of the azeotropic point of the VLE diagram (see Figure 4). The composition profiles provide strong evidence that the number of trays is over-projected for the experimental conditions tested. Indeed, in some of the stages the enrichment of vapor phase in aniline is quite small, thus leading to the conclusion that the column can successfully separate a higher flow of feed stream (with a similar composition) with the same efficiency, provided the heat supplied to the reboiler increases and flooding does not occur.

Figure 6 shows that the liquid and vapor flows across the column are approximately constant in the enrichment and

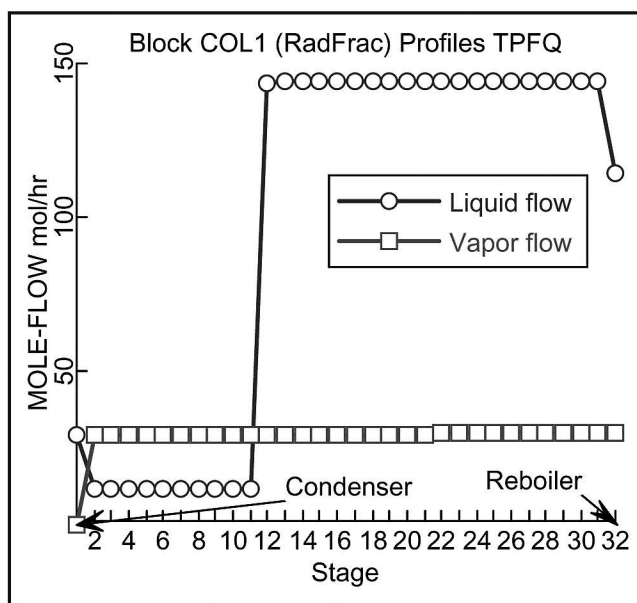


Figure 6. Liquid and vapor flows across the column.

stripping zones. Since stage 11 (12 in Figure 6) is the feed stage and the state of the stream is saturated liquid, the liquid flow rate in the stripping zone is increased by an amount equal to the feed flow rate. These conditions enable the McCabe-Thiele graphical construction^[13] to be used to estimate the number of theoretical trays required to perform the separation. Typical values achieved by students are about 14 trays plus the condenser and the reboiler.

CONCLUSIONS

Operating a laboratory distillation column is a good experiment for demonstrating the application of some concepts of unit operations, vapor-liquid equilibrium prediction, and process simulation. The experiment described in this paper embraces a wide range of topics including process control, chemical analysis, and numerical methods for handling rigorous distillation models. It also enables students to gain experience in operating and controlling a distillation unit. Moreover, the results provide the research community with sufficient evidence to support the validation of the equilibrium stage model for the heterogeneous azeotropic system formed by aniline and water. The results show that the column is too large for the experimental conditions tested, and additional knowledge regarding its behavior can be acquired if the inlet flow is increased and digital temperature meters are installed in each tray to validate the temperature profile. But the experiment might be successfully applied to other azeotropic systems, such as a benzene-mononitrobenzene-water mixture.

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APPENDIX

AspenPlus Input Summary file

Input Summary created by AspenPlus Rel. 11.1 at 18:15:48

Sat., Jan. 28, 2006.

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&
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  JMETH=INIT &
  LL-METH=GIBBS NPHASE=2 DAMPING=NONE
  COL-CONFIG CONDENSER=TOTAL REBOILER=KETTLE
  FEEDS FEED 12 ON-STAGE
  PRODUCTS RESID 32 L / DESTIL 1 L
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  COL-SPECS QN=335. MOLE-D=17.72 <mol/hr>
14
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  0.92 / 6 0.92 / 7 0.92 / 8 0.92 / 9 0.92 / 10 &
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 372.6 / 6 372.6 / 7 372.6 / 8 372.6 / 9 372.6 / &
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8.997E-006 / 23 8.998E-006 / 24 8.999E-006 / 25 &
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 29 9E-006 / 30 9E-006 / 31 9E-006
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 EO-CONV-OPTI
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 SENTENCE=RESULTS
 DEFINE Z2 BLOCK-VAR BLOCK=C1 VARIABLE=VRATE &
 SENTENCE=PROFILE ID1=2
 TABULATE 1 "Z1"
 TABULATE 2 "Z2"
 VARY BLOCK-VAR BLOCK=C1 VARIABLE=QN SENTENCE=COL-
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 DEFINE Z2 BLOCK-VAR BLOCK=C1 VARIABLE=VRATE &
 SENTENCE=PROFILE ID1=2
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 TABULATE 2 "Z2"
 VARY MASS-FLOW STREAM=FEED SUBSTREAM=MIXED
 COMPONENT=ANILINE
 RANGE LOWER="5.0E-6" UPPER="4.0E-5" INCR="2.5E-6"
 CONV-OPTIONS
 PARAM TEAR-METHOD=NEWTON SPEC-LOOP=INSIDE
 STREAM-REPOR MOLEFLOW MASSFLOW
 PROPERTY-REPCES NOPARAM-PLUS □