PRODUCT COMPOSITION CONTROL OF A PRESSURE SWING DOUBLE COLUMN BATCH RECTIFIER

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Abstract

The pressure swing separation of a binary maximum azeotrope (water-EDA) in a double column batch rectifier is studied by rigorous simulation. For controlling the product compositions a simple scheme is presented. On the basis of temperatures of the top products PID controllers manipulate their flow rates varying the reflux ratios. The influence of the most important operational parameter (division ratio for the stream leaving the common bottom vessel) is investigated. For rigorous simulation calculations a professional dynamic flowsheet simulator is applied.

**Keywords:** pressure swing, batch rectification, maximum azeotrope, control.

Introduction

Binary pressure sensitive azeotropes can be separated by pressure swing distillation (PSD). Continuous PSD was first applied in the industry in 1928. Phimister and Seier[5] studied first the batch (stripping) and semicontinuous application of PSD by simulation. First Repke et al.[6] investigated experimentally the batch PSD (PSBD, pilot-plant experiments for the separation of a minimum azeotrope in a batch rectifier (BR) and stripper (BS)). Modla and Lang[2] studied different batch configurations (BR, BS, combination of BR and BS and middle vessel column(MVC)) by feasibility studies and rigorous simulation for the separation binary (max. and min.) homoazeotropes. By modifying the MVC, which has not been proven suitable for the PSBD, they suggested two new double column batch configurations: rectifier (DCBR, Fig. 1a) and stripper (DCBS, Fig. 1b). They compared the different configurations for a given set of operational parameters without optimisation and control. For minimum azeotropes the best results (minimal specific energy consumption for the same quality products) were obtained with the DCBS and for maximum azeotropes with the DCBR, respectively. The columns of these configurations can be operated practically in steady state. Kopasz et al.[1] suggested a simple scheme for the composition control of a DCBS investigating the separation of a maximum azeotrope. Modla et al.[3] studied the feasibility of batch PSD separation in one and two column configurations of most frequent types of ternary homoazeotropic mixtures.

When operating these new configurations the liquid composition of the common vessel of the two columns must be kept between the two azeotropic compositions. The ratio of two product flow rates of can be changed by varying the reboil (DCBS)/reflux (DCBR) ratios and/or the ratio of division of the stream leaving the common vessel. In the case of the DCBS this ratio determines the ratio of the liquid flow rates, whilst in the case of the DCBR that of the vapour flow rates (and heat duties) of the two columns, respectively. The goals of this paper are:

-investigation of the influence of the main operational parameters in case of DCBR,
-determination of optimal value of operational parameters (providing the prescribed separation with minimal energy consumption),
-to propose an appropriate scheme for product composition control of this new configuration.

The calculations were made for the mixture water-EDA by using a professional dynamic simulator (CCDCOLUMN). The temperature-composition (T-x,y) diagrams and azeotropic data of the mixture studied are shown for the two different pressures in Fig. 2 and Table 1, respectively. We can conclude that the difference of the two azeotropic compositions is much more than 5 mole %, while the difference of the two pressures applied is less than 10 bar, so the pressure swing process can be economical for the separation by Perry et al.[4].

a. DCBR   b. DCBS
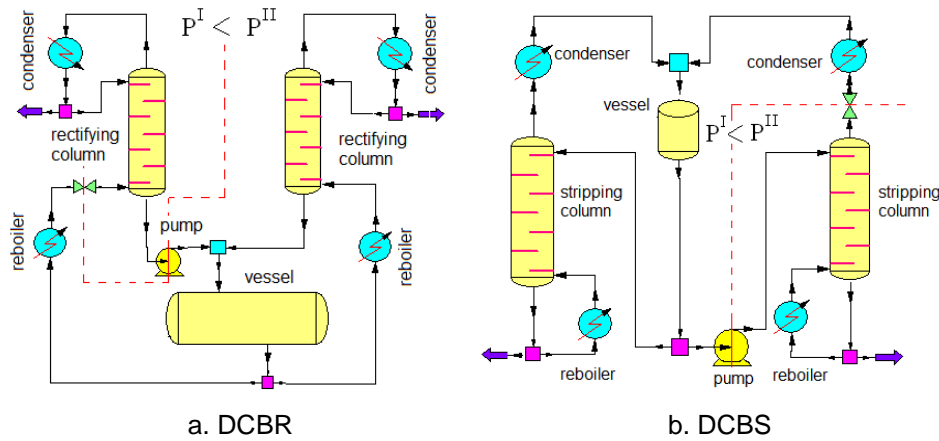
Figure 1. The scheme of a Double Column Batch Rectifier and Double Column Batch Stripper
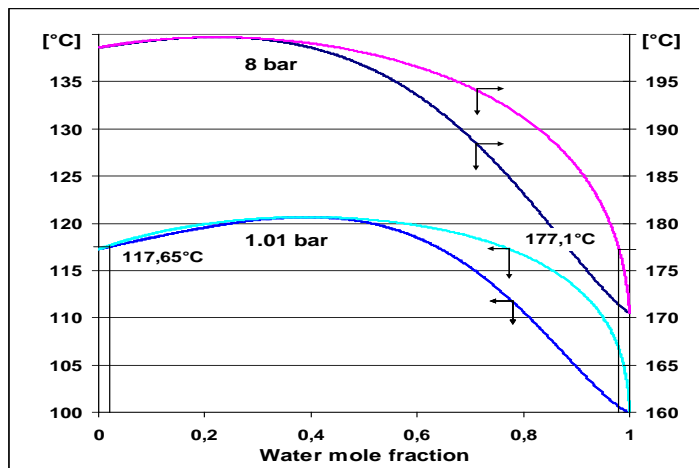
Figure 2. T-x,y diagrams of water-EDA

Component		water(A)	EDA(B)
P	[bar]	1.01	8.00
	x_{az}	0.39	0.22
T_{az}	[°C]	120.6	199.7
$T_{BP,A}$	[°C]	100.0	170.5
$T_{BP,B}$	[°C]	117.3	198.6

Table 1. Azeotropic data (UNIQUAC parameters:-19.6564,-790.52 cal/mol)

2. Simulation method

The following simplifying assumptions were applied:

- theoretical stages,
- negligible vapour hold-up,
- constant volumetric liquid plate hold-up.

The model equations to be solved are well known:

a. Non-linear differential equations (material balances, heat balances),
b. Algebraic equations (vapour-liquid equilibrium (VLE) relationships, summation equations, hold-up equivalence, physical property models).

For solving the above model equations we used the CCDCOLUMN dynamic flow-sheet simulator (ChemCad 6.0) applying the simultaneous correction method. The following modules were used: DYNCOLUMN (column sections), DYNAMIC VESSEL (top vessel and product tanks), HEAT EXCHANGER, PUMP, VALVE, MIXER, DIVIDER, CONTROLLER, CONTROL VALVE. The ChemCad model of the double column batch rectifier with control of product compositions is shown in Fig. 3.
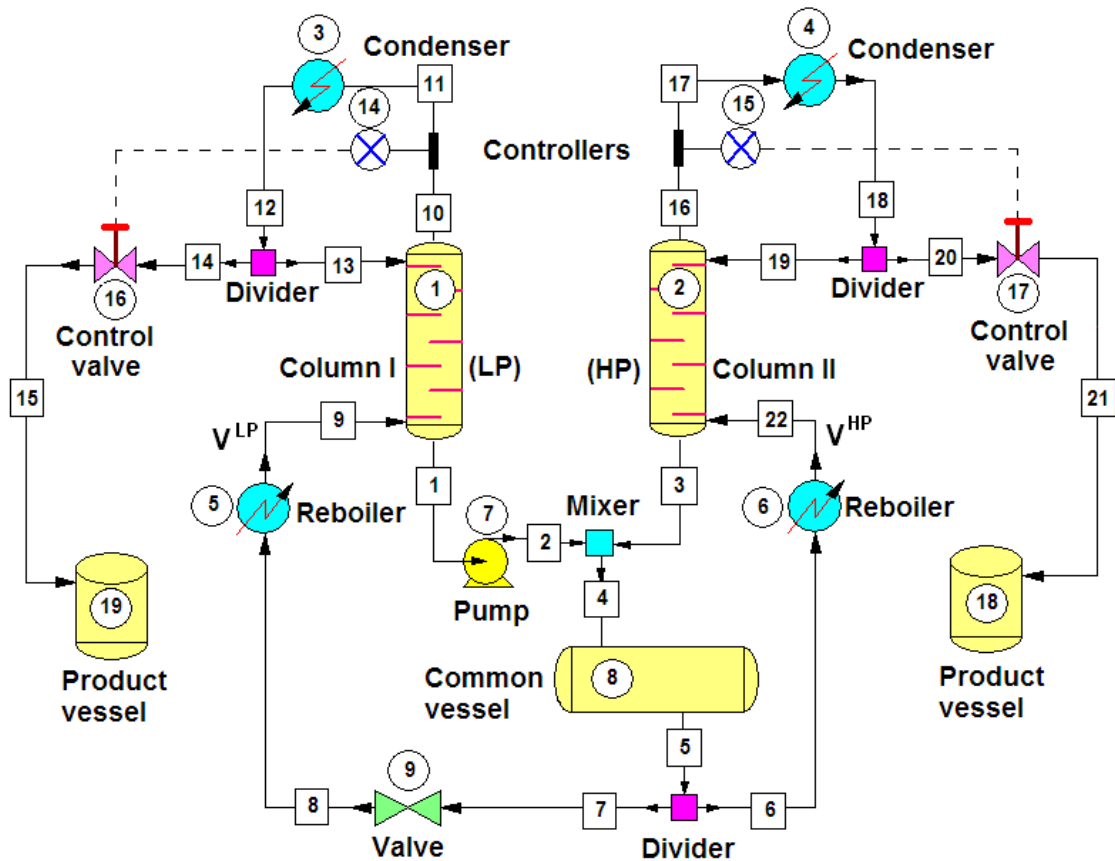
Figure 3. ChemCad model of the double column batch rectifier with control loops.

3. Results

The number of theoretical stages for each column sections is 40. (The total condenser and total reboiler do not provide a theoretical stage.) The pressure of the columns: P^{LP}=1.01bar and P^{HP}=8 bar. The liquid hold-up is 2 dm^3/plate. The total flow rate of liquid leaving the common vessel (divided between the two columns and then totally vapourised): 6 m^3/h = 184.2 kmol/h. The quantity of charge (including the two column hold-ups) containing 30 mol% EDA is 84.44 kmol (2.7505 m^3). The prescribed purity is 98 mol% for both products. The reflux ratios R^{LP} and R^{HP} are changed by PID controllers manipulating (with linear control valves) the top product flow rates (D^{LP} and D^{HP}), respectively. At the start of the distillation plates of the columns are wet (they are filled with charge at its boiling point at the given pressure). The whole process is finished when the amount of liquid in the vessel decreases to 0.8 kmol.

First, the parameters of the two PID controllers (A_P=1/PB, T_I and T_D) providing stable, good quality control of the product compositions in the whole region of division ratio ($\varphi=V^{LP}/(V^{LP}+V^{HP})$) studied are determined. Then, the influence of this operational parameter on the performance of the DCBR is studied and its optimum value yielding the minimal overall specific heat energy consumption ((SQ^{LP}+ SQ^{HP})/(SD^{LP}+ SD^{HP}) is determined. (We consider SQ^{LP} és SQ^{HP} as the summation of the absolute value of the heating input energy in the reboiler and the cooling output energy in the condenser. The energy consumption of the pumps is neglected besides the heat energy consumption of the process, since it is lower by more than one order of magnitude.)

3.1 Tuning of PID controllers

Our aim is to determine a set of parameters (A_P=1/PB, T_I and T_D) of the PID controllers which provide good quality control of product compositions in the whole region of the division ratio ($\varphi=V^{LP}/V_{total}$) by taking into consideration the usual criterions (maximal overshoot, control time, number of oscillations). The controllers are calculated by the standard PID algorithm, which is the base setting in the ChemCAD. (The error definition is reverse which means: Error = X_{set} – X.)

The quality of control is determined by the evolution of not the controlled variables (temperature of the two top products) but the position of the two control valves (varying the flow rate of the two top products). This was made because the valve position (%) varies much more rapidly than the controlled variable. The following criteria of quality of control are prescribed concerning the two control valves: maximal overshoot: 33 %, maximum number of oscillations during the settling time T_S (within an error band of +- 5 %): 3. We gave as setpoints the temperatures, belonging to the purities of 98 mol% (*Fig. 2).* (The relation between the composition and the temperature is non-linear.)

Table 2. Parameters and quality data of control for an appropriate tuning

a. PID parameters:

	PB, %	T_I, min	T_D, min	Set point,°C
Column I	7	20	0	117.65
Column II	20	20	0	177.18

b. Sensor equation terms:

	Variable min., °C	Variable max., °C	Control input min., mA	Control input max., mA
Column I	110	130	4	20
Column II	150	200	4	20

c. Valve flow coefficients: $K_{v,I}$= 1, $K_{v,II}$=0.1

d. Control quality data:

	Column I	Column II
Maximal overshoot (valve %):	(40-30)/30=0.33	(33-27)/27= 0.22
Settling time (T_s), min:	20	15
No. of oscillations within T_S:	2	2

For the selected control parameters the evolution of the position of the control valves, distillate compositions and reflux ratios is shown in Fig. 4. (Table 2 contains the parameters of PID controllers and control quality data.) With the above values of the PID controller parameters we were able to produce prescribed purity products for a long period, when the top temperatures were also constant. At the start of the process for a shorter time the product purities exceeded their prescribed values. The valve positions after two oscillations became provisionally constant (T_s and the maximal overshoot were determined for this period), then they showed slow, monotonous variations. (The evolution of the reflux ratios show similar behaviour, but the direction of the variation is just the opposite.)

3.2 Influence of the division ratio
The (vapour) division ratio determines the vapour flow rates in the two columns. It influences the reflux ratios which are necessary for producing the prescribed purity distillates in both columns. (The higher the reflux ratio the lower the distillate flow rate.) The duration of the process depends on the distillate flow rates and so on the division ratio. Hence the division ratio influences the specific heat energy consumption, as well.

The vapour division ratio is varied in the region 0.3-0.7. The specific energy consumption is minimal at φ=0.475 (Fig. 5). Prescribed purity products are obtained with good recovery (Table 3). This table contains also the most important results for the process, such as the total and specific heat energy consumptions of the production. It must be still noted the recoveries could be still slightly increased by emptying totally the common vessel. In the case studied we were able to practically empty the vessel while maintaining the prescribed purities in the product tanks. However under a certain amount of residue (0.8 kmol) the operation of the control loops became unstable (oscillation of the position of control valves).
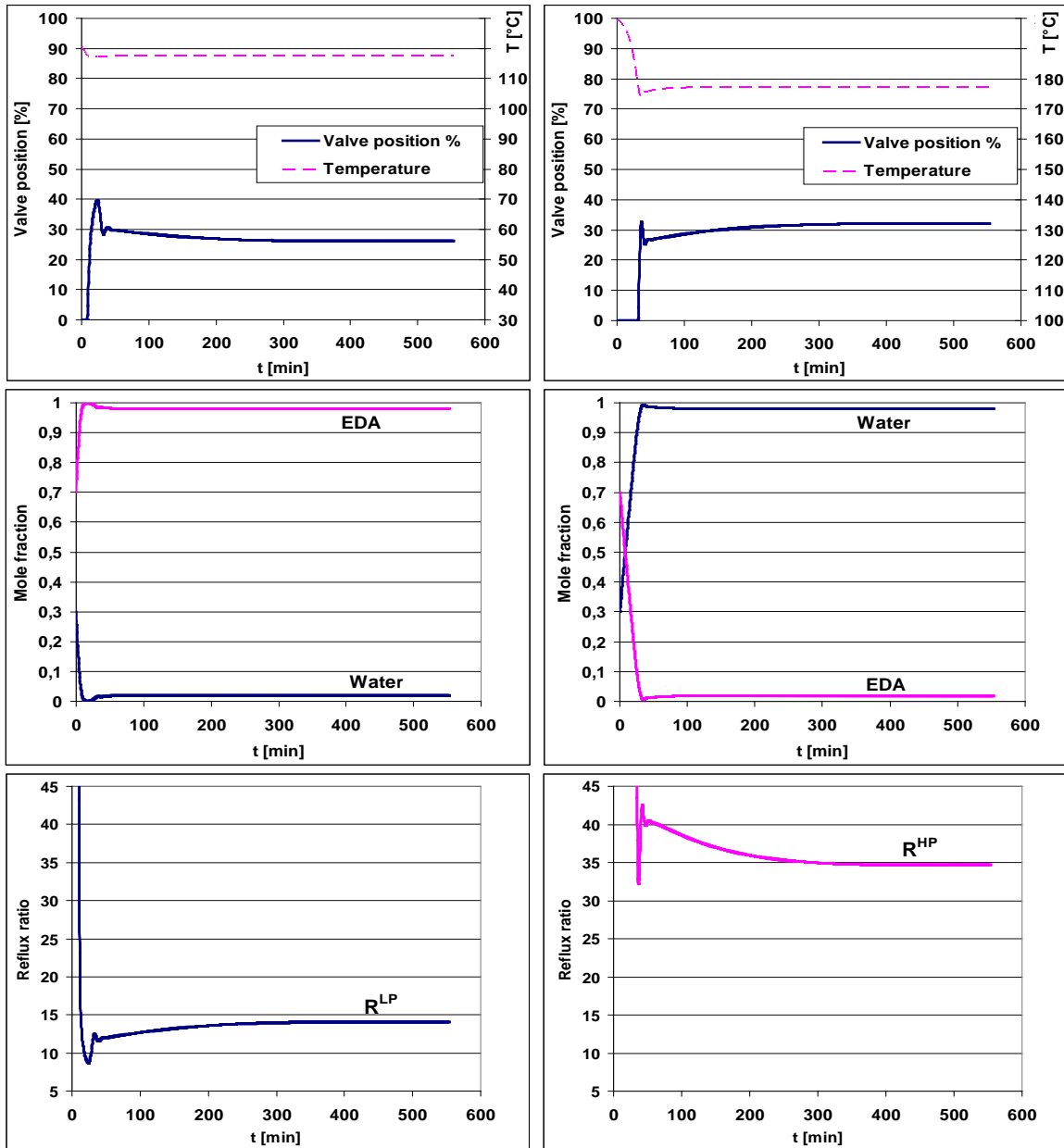
a. Column I (LP)   b. Column II (HP)

Fig. 4. The evolution of control valve positions and head temperatures
(a), distillate compositions (b), reflux ratios (c) at φ=0.475.
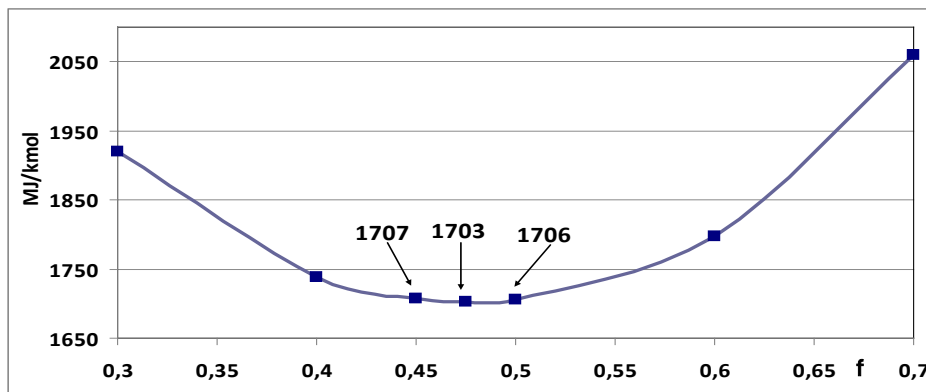
Fig. 5. The influence of the vapour division ratio on the specific energy consumption

Table 3. Most important results of the production for the optimal division ratio

Water recovery	%	86.8
EDA recovery	%	93.2
Water purity	mol %	98.12
EDA purity	mol %	98.07
Total energy (SQ)	MJ	68,926
Specific energy: $SQ/(SD_A + SD_B)$	MJ/kmol	1703
Production time	min	563

Conclusion

We investigated the separation of a maximal boiling point azeotropic mixture (water-EDA) in a double column batch rectifier (DCBR) with rigorous simulation by applying the dynamic module of a professional flowsheet simulator ChemCad (CCDCOLUMN). For controlling the product compositions a simple scheme was suggested. A potential set of PID parameters was determined, wherewith the prescribed purities were satisfied and good recoveries were obtained. We investigated the influence of the most important operational parameters (ratio of the vapour flows of the two columns) on the performance of the process, and determined its optimum value providing the minimal overall specific heat energy consumption.

Acknowledgement

References

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