

PRODUCT COMPOSITION CONTROL OF A NEW BATCH PRESSURE SWING RECTIFYING SYSTEM

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When operating the Double Column Batch Stripper (DCBS) configuration the liquid composition of the common vessel of the two columns must be kept between the two azeotropic compositions by affecting the flow rates of the two products. These can be varied by changing the reboil ratio and/or ratio of division of the liquid flow leaving the common vessel.

The goals of this paper:

- to propose and study a simple control scheme with PID parameters (providing good quality of control) for the new configuration,
- investigation of the influence of the liquid division ratio,
- determination of optimal value of liquid division ratio (providing the prescribed separation with minimal specific energy consumption).

The calculations were made for a minimum (n-pentane – acetone) azeotropic mixture by using a professional dynamic simulator (CCDCOLUMN). By the aid of a PID controller we modified the flow rate of the bottom products (affecting the reboil ratios of the columns). We investigated the action of the control loops and the system for two different set points. In the first case the composition of the bottom products, in the second one – most common in the industry – the bottom temperatures were kept constant.

Keywords: batch rectification, pressure swing, minimum azeotrope, composition 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 Seider (2000) studied first the batch (stripping) and semicontinuous application of PSD by simulation. First Repke et al. (2007) 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 (2008) 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 (maximum and minimum) homoazeotropes.

The different pressures can be separated:

- in time → one column section (e.g. BR, BS)
- in place → two column sections (e.g. MVC)

By modifying the MVC, which has not been proven suitable for the PSBD, they suggested two new double column batch configurations: rectifier (DCBR) and stripper (DCBS, Fig. 1).

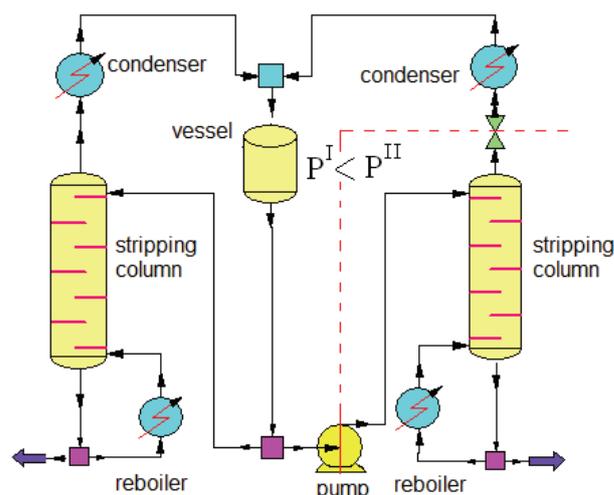


Figure 1: The scheme of a DCBS

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. Modla et al. (2010) studied the feasibility of batch PSD separation 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 a DCBS can be changed by varying the /reboil ratios and/or the ratio of division of the liquid flow leaving the common vessel.

The goals of this paper are:

- to investigate the operation of the DCBS for the separation of a minimum azeotrope,
- to study a simple scheme for the control of product compositions (directly the composition or temperatures of bottoms product are controlled and their flow rates are manipulated),
- to investigate the effects and to determine the optimal value of the liquid division ratio.

The calculations were made for the mixture n-pentane-acetone 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.

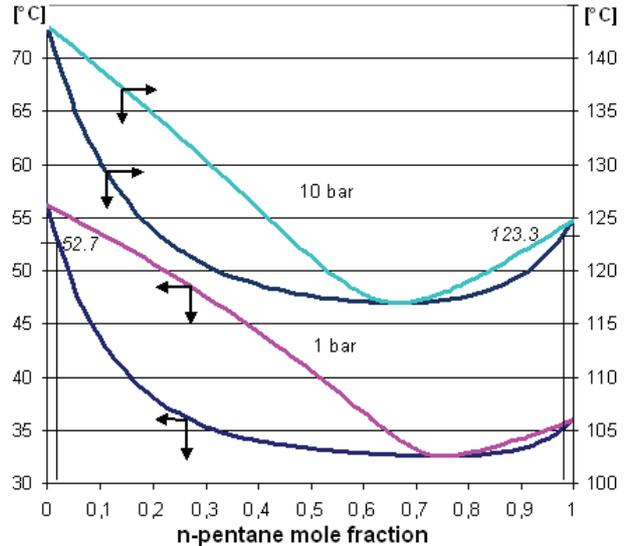


Figure 2: T-x,y diagrams of n-pentane-acetone

Table 1: Azeotropic data (UNIQUAC parameters: 571.98 and 95.033 cal/mol)

Component	pentane(A)	acetone(B)
P [bar]	1.01	10.0
x_{az}	0.754	0.668
T_{az} [°C]	32.5	116.9
$T_{BP,A}$ [°C]	36.0	124.7
$T_{BP,B}$ [°C]	56.2	142.9

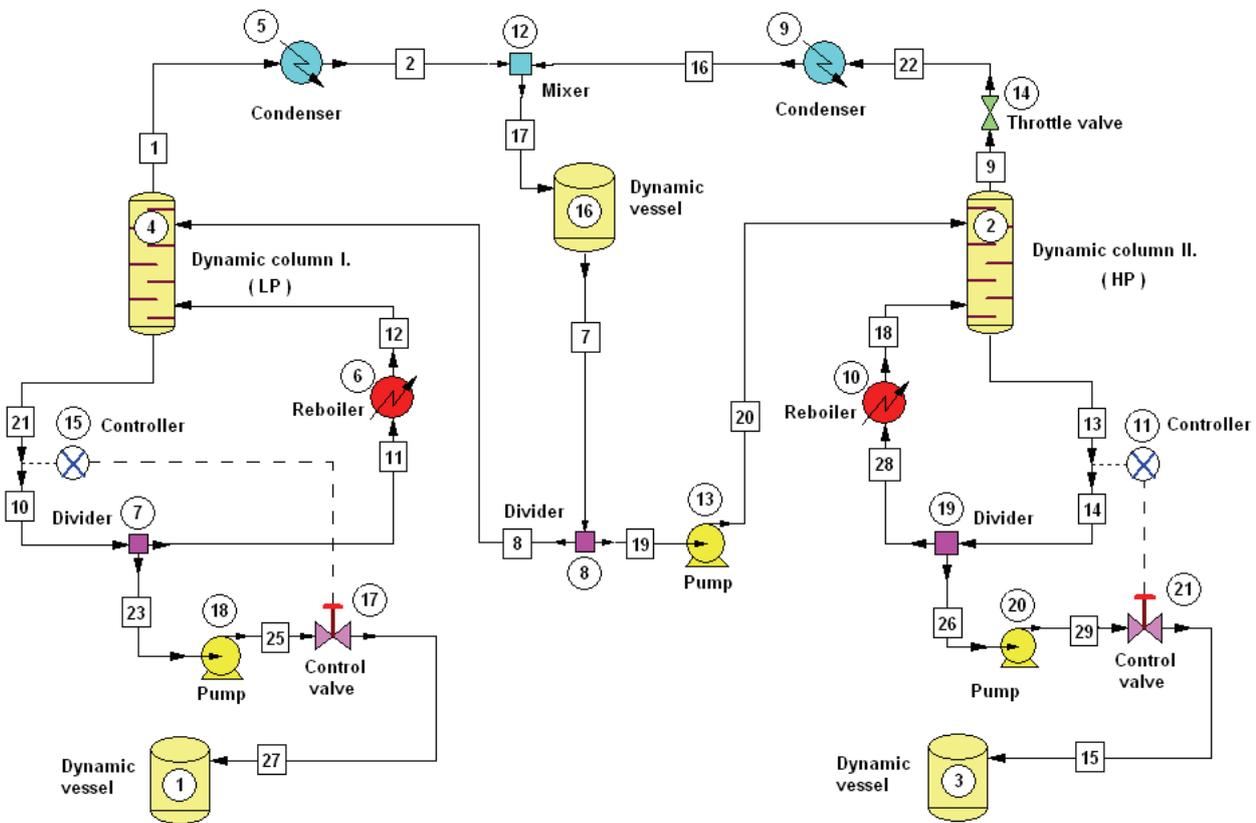


Figure 3: ChemCad model of the double column batch stripper with control loops

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 of ChemCad 6.0 (Chemstations 2006,). For the simulation of columns simultaneous correction method was applied.

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 stripper with control of product compositions is shown in *Fig. 3*.

Simulation 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 liquid hold-up is $2 \text{ dm}^3/\text{plate}$. the pressure of the columns: $P^{\text{LP}} = 1.013 \text{ bar}$ and $P^{\text{HP}} = 10 \text{ bar}$.

The total flow rate of liquid leaving the common vessel: $L_{0,\text{total}} = L_0^{\text{LP}} + L_0^{\text{HP}} = 6 \text{ m}^3/\text{h}$. 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, "wet start-up").

The quantity of charge containing 30 mol% pentane filled into the common vessel is 4.022 kmol (0.471 m^3). The prescribed purity is 98 mol% for both products. The reboil ratios R_s^{LP} and R_s^{HP} are changed by PID controllers manipulating (with linear control valves) the product flow rates W^{LP} and W^{HP} , respectively. The whole process is finished when the amount of liquid in the vessel decreases to 12.5% of the charge.

Tuning of PID controllers

Our aim is to determine a set of parameters (A_P , T_I and T_D) of the PID controllers which provide good quality control of product compositions in the whole region of the liquid division ratio ($\varphi = L_0^{\text{LP}}/L_{0,\text{total}}$) 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: $\text{Error} = X_{\text{set}} - X$.)

The quality of control is determined by the evolution of not the controlled variables (composition or temperature of the two bottoms products) but the position of the two control valves (varying the flow rate of the two bottoms product). This was made because the valve position (%) varies much more rapidly than the controlled variable. The following criteria of quality of control are given concerning the two control valves:

- maximal overshoot: 33%,
- maximum number of oscillations during the settling time T_S (within an error band of $\pm 5\%$): 3.

We investigated the control schemes with two methods from the point of view of the setpoint parameter. In our first calculations we gave into the program bottom-composition-setpoint, and tried to maintain the purity of the bottom product around 98 mol% with the PID controllers. Then 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 contains the parameters of PID controllers and sensors. The control quality data for the two different cases are shown in *Tables 3* and *4*.

Table 2: Set of parameters for composition and temperature control

Control mode	Composition		Temperature	
	Column I	Column II	Column I	Column II
PB, %	80	50	45	120
T_b , min	2.5	10	13	3
T_D , min	0	1	0.5	1
Setpoint	0.982	0.98	52.7	123
Variable minimum	0.8	0.6	50	117.1
Variable maximum	1	1	56.15	124.74
Ctrl input minimum	4	4	4	4
Ctrl input maximum	20	20	20	20

Table 3: Control quality data for composition control

	Column I	Column II
Maximal overshoot, %	8	11
T_s , min	20.5	15.0
No. of oscillations within T_s	2	1

Table 4: Control quality data for temperature control

	Column I	Column II
Maximal overshoot, %	33	32
T_s , min	6.75	7.75
No. of oscillations within T_s	1	1

Influence of the liquid division ratio

After tuning the PID controllers we investigated the effect of the liquid division ratio (φ) on the process.

The optimal value of φ was determined according to the minimal overall specific energy consumption $(SQ^{LP} + SQ^{HP}) / (SW^{LP} + SW^{HP})$. 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 power-supply of the pumps was disregarded, because it's order of magnitude is much more smaller than the heating energy. The liquid division ratio was varied in the region 0.3–0.9. The specific energy consumption is minimal at $\varphi = 0.55$ (Fig. 4) in both cases of control mode (composition control, temperature control).

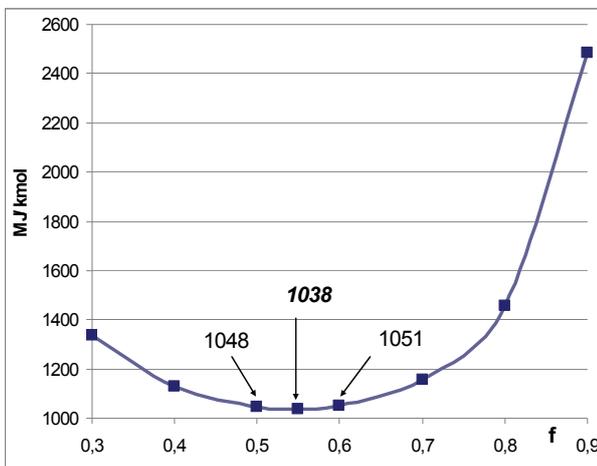


Figure 4: The influence of the liquid division ratio on the specific heat energy consumption $(SQ / (SW_A + SW_B))$

Prescribed purity products are obtained with acceptable recoveries (Table 5). This table contains also the most important results for the process, such as the total and specific heat energy consumptions of the production. It's worthy of note that the recoveries can be increased by the reduction of the amount (12,5% of the starting value) remaining in the common vessel.

During our investigations we were able to empty the common vessel totally ensuring the prescribed product purities, however under 12% the operation of the controllers became unstable (oscillations).

Fig. 5 shows the evolution of control valve positions and bottom temperatures, bottoms compositions, reboil ratios at the liquid division ratio of $\varphi = 0.55$.

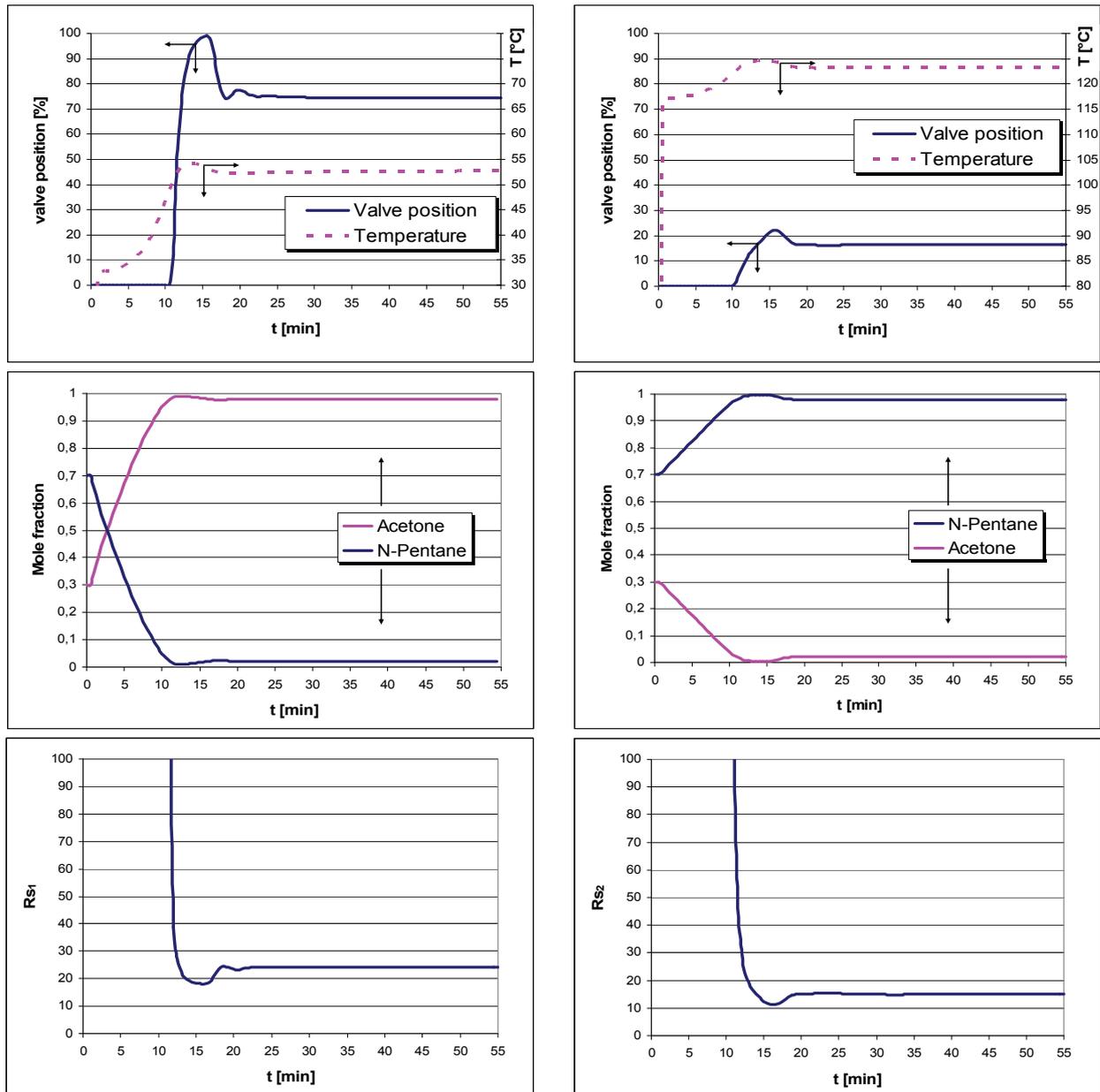
Table 5: Most important results of the production for the optimal liquid division ratio

Control mode	composition	temperature	
N-pentane recovery*	%	86.50	75.32
Acetone recovery*	%	79.50	67.54
N-pentane purity	mol%	98.65	98.20
Acetone purity	mol%	97.96	98.03
Total calorific energy (SQ)	MJ	3517	3106
Specific calorific energy: $SQ / (SW_A + SW_B)$	MJ/mol	1019	1038
Production time	min	62.5	54.0

* related to the amount filled into the comon vessel at the start

Conclusion

We investigated the separation of a maximal boiling point azeotrope n-pentane-water in the double column batch stripper (DCBS) with rigorous simulation by applying the dynamic module of a professional flowsheet simulator ChemCad (CCDCOLUMN). A potential set of PID parameters was determined, wherewith both the prescribed purities and the prescribed criteria of control quality were satisfied. We investigated the influence of the liquid division ratio on the performance of the process, and determined its optimum value (looking for the minimal overall specific heat energy consumption). We got similar results for the value of the minimal overall specific energy consumption in both cases (composition control, temperature control, which is applied most commonly in the industry).



Column I (LP)

Column II (HP)

Figure 5: The evolution of valve positions and bottom temperatures, bottom compositions, reboil ratios at $\phi = 0.55$

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