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Operation and Composition Control of a New Pressure Swing Batch Distillation System

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Abstract

The pressure swing separation of a binary minimum azeotrope (n-pentane-acetone) in a double column batch stripper is studied by rigorous simulation. For controlling the product compositions a simple scheme is presented. On the basis of temperatures of bottoms product PID controllers manipulate their flow rates varying the reboil ratios. The controllers are tuned. The influence of the most important operational parameter (division ratio of liquid leaving the common top vessel) is investigated. For rigorous simulation calculations a professional dynamic flowsheet simulator is applied.

Keywords: batch stripping, pressure swing, minimum azeotrope, control.

1. 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 (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 min. 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. (2009) 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.

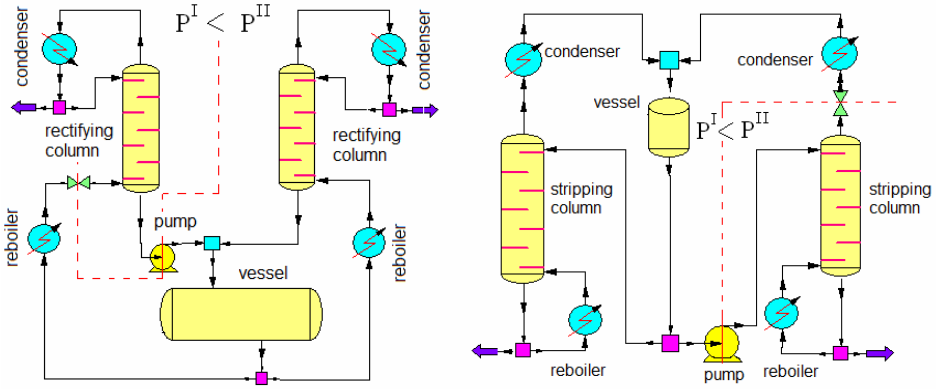
The goals of this paper are:

-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 (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).



a. DCBR *b. DCBS*

Figure 1. The scheme of a DCBR and DCBS

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.

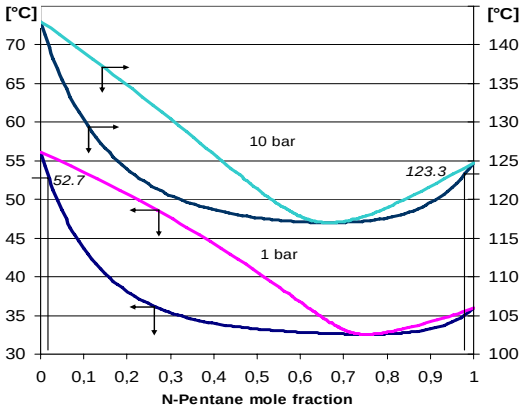


Figure 2.T-x,y diagrams of n-pentane-acetone

Component	pentane(*A*)	acetone(*B*)
P [bar]	1.01	10
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

Table 1. Azeotropic data (UNIQUAC parameters: 571.98 and 95.033 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). 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*.

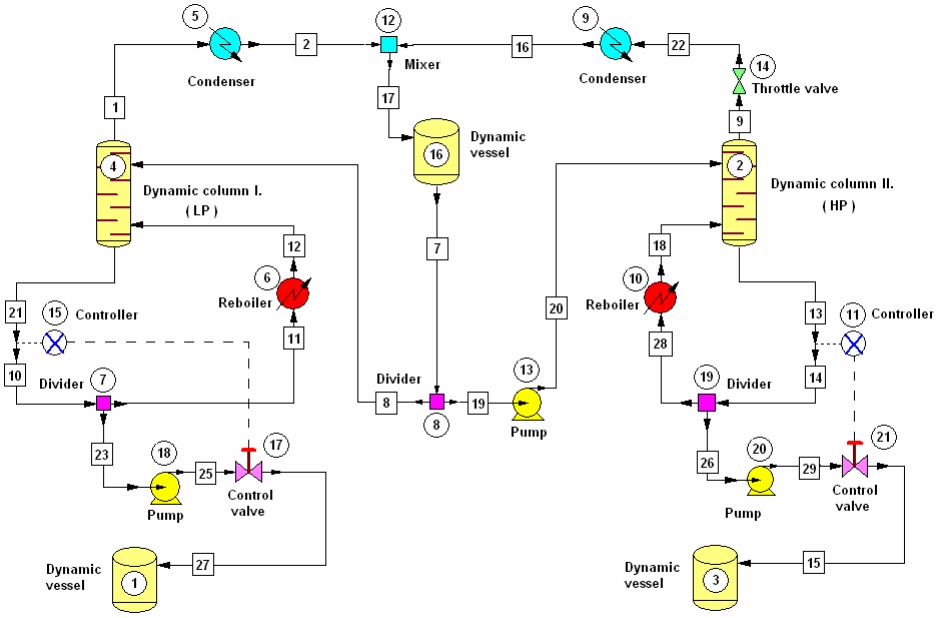


Figure 3. ChemCad model of the double column batch stripper with control loops.

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 liquid hold-up is 2 dm3/plate. the pressure of the columns: P^{LP}=1.013 bar and P^{HP}=10 bar. 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 total flow rate of liquid leaving the common vessel: $L_{0,total}$ = L_0^{LP}+ L_0^{HP} = 6 m^3/h. The quantity of charge containing 30 mol% pentane is 4.022 kmol (0.471 m3). 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.
First, the parameters of the two PID controllers (A_P, T_I and T_D) providing stable, good quality control of the product compositions in the whole region of liquid division ratio

($\phi=L_0^{LP}/L_{0,total}$) studied are determined. Then, the influence of this operational parameter on the performance of the PSBS is studied and its optimum value yielding the minimal overall specific energy consumption ($(SQ^{LP}+SQ^{HP})/(SW^{LP}+SW^{HP})$) is determined.

3.1. Tuning of PID controllers

Our aim is to determine a set of parameters of the PID controllers which provide good quality control of product compositions by taking into consideration the usual criterions (maximal overshoot, control time, number of oscillations).

The quality of control is determined by the evolution of not only the controlled variables (temperature of the two bottoms products) but also that of the position of the two control valves (varying the flow rate of the two bottoms product). 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 +-5 %): 3.

In *Fig. 4* the evolution of the position of the control valve and bottoms composition of Column I for an inappropriate set of controller parameters is shown. (Both the position of the control valve and the controlled variable show oscillations without damping.)

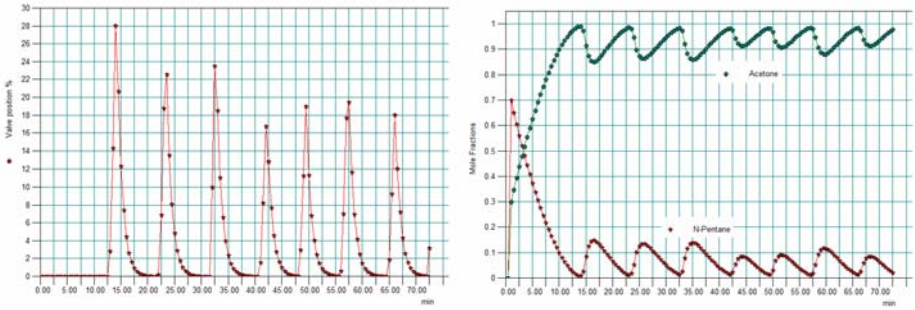


Figure 4. The evolution of the position of the control valve and bottoms composition for an inappropriate setting of PID parameters (Column I, PB=10 %, T_I= 1 min, T_D= 0)

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

a. PID parameters:

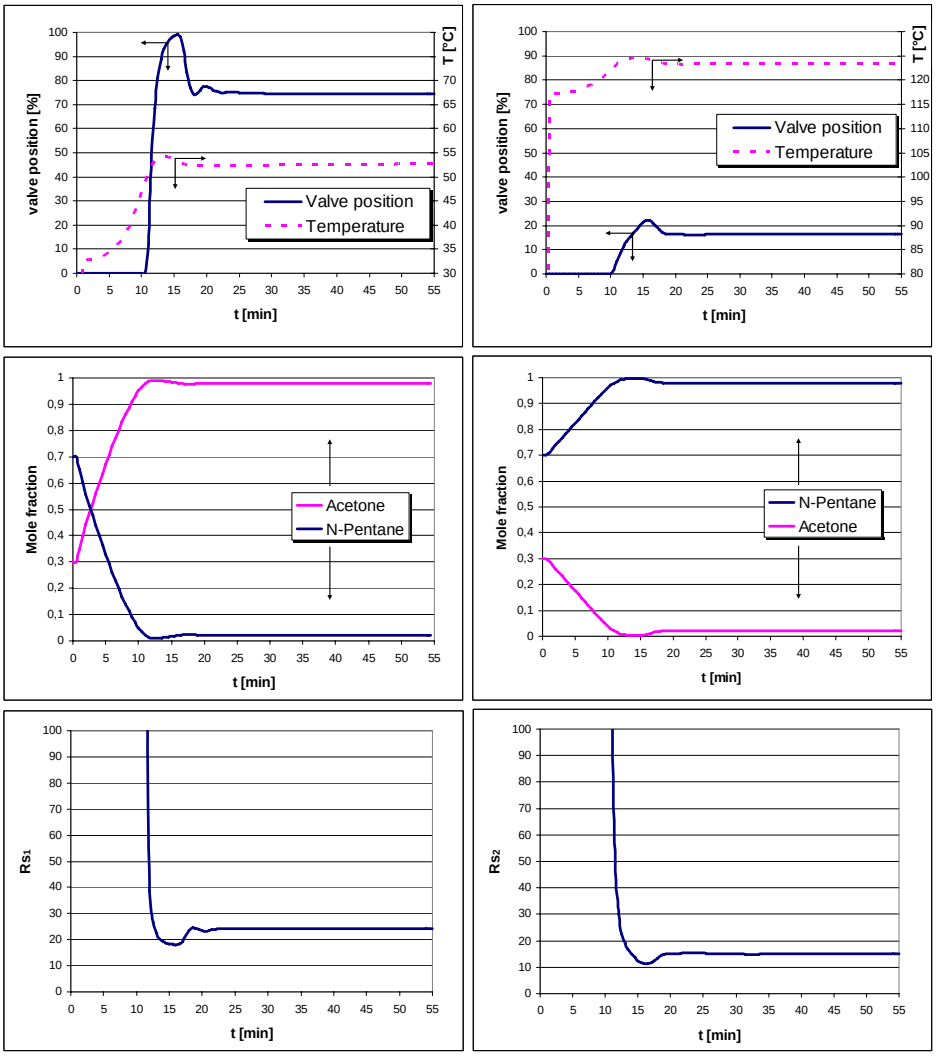
	PB, %	$T_{I,}$ min	$T_{D,}$ min	Set point,°C
Column I	45	13	0.50	52.7
Column II	120	3	1	123.3

b. Valve flow coefficients: K_v^I= 0.13 K_v^{II}=2

c. Control quality data:

	Column I:	Column II:
Maximal overshoot:	(99.13-74.45)/74.45=**0.33**	(21.97-16.64)/)/16.64=**0.32**
Settling time, min:	17.25-10.5=**6.75**	17.75-10=**7.75**
No. of oscillations within T_S:	1	1

For the controller parameters selected (*Table 2*) the evolution of the position of the control valves, bottoms compositions and reboil ratios is shown in *Fig. 5*. (*Table 2* contains the control quality data, as well.)



a. Column I *b. Column II*

Fig. 5. The evolution of control valve positions and bottom temperatures (a), bottoms compositions (b), reboil ratios (c) (ϕ=0.55)

3.2. Influence of the liquid division ratio

The liquid division ratio is varied in the region 0.3-0.9. The specific energy consumption is minimal at ϕ=0.55 (*Fig. 6*). Prescribed purity products are obtained with reasonable recovery (*Table 3*). This table contains also the most important results for the process, such as the total and specific energy consumptions of the production. It must be

still noted that the recoveries could be still increased by reducing the quantity of residue in the common top 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 (12 % of the charge) the operation of the control loops became unstable, therefore we stopped the process.

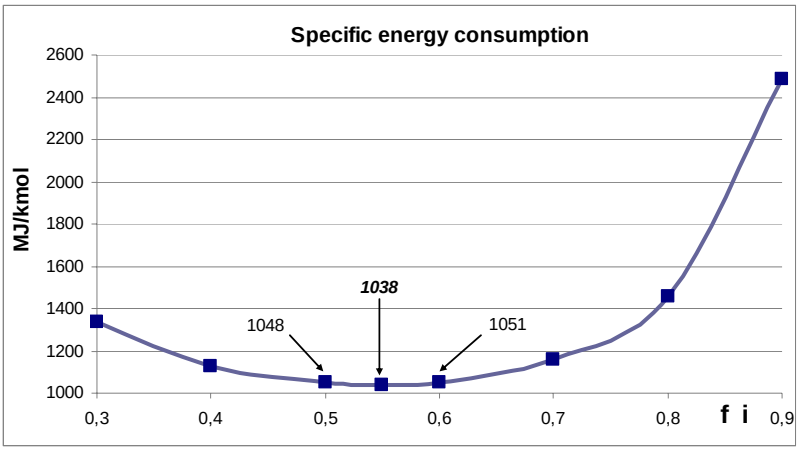


Fig. 6. The influence of the liquid division ratio on the specific energy consumption

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

N-pentane recovery	%	75.32
Acetone recovery	%	67.54
N-pentane purity	mol %	98.20
Acetone purity	mol %	98.03
Total energy (SQ)	MJ	3106
Specific energy: $SQ/(SW_A + SW_B)$	MJ/mol	1038
Production time	min	54

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