NEW COLUMN CONFIGURATIONS FOR PRESSURE SWING BATCH DISTILLATION II. RIGOROUS SIMULATION RESULTS

Modla G. and P. Láng*

Budapest University of Technology and Economics, Department of Process Engineering, H-1521 Budapest, Muegyetem rkp. 3-5
www.vegyelgep.bme.hu, *lang@mail.bme.hu

Objective: to verify the conclusions of the feasibility studies, to investigate the performance of the different feasible configurations and to compare them with rigorous simulation calculations.

INTRODUCTION

Distillation is the separation method most frequently applied in the chemical industry, which is based on the difference of volatility of the components of a liquid mixture. For the separation of the two components (***A*** and ***B***) forming an azeotrope a special distillation method must be applied such as the pressure swing distillation, extractive or heteroazeotropic distillation.

Batch distillation has always been an important part of seasonal, uncertain or low capacity and high-purity chemicalsô production. It is a process of key importance in the pharmaceutical and several other industries and in the regeneration of waste solvent mixtures. Modla and Lang (2007) studied the feasibility of pressure swing batch distillation of binary mixtures (forming minimum or maximum azeotrope) in different column configurations assuming maximal separation. They suggested two novel configurations double column batch rectifier (DCBR) and double column batch stripper (DCBS). We stated that these new configurations may provide a lot of advantages against the well-known simpler configurations (batch rectifier(BR) or stripper(BS)). We also studied the alternate application of a rectifier and a stripper (BR-BS), which can be applied for both minimum and maximum azeotropes.

In the practice we can not produce maximal separation since
-the number of stages is limited,
-the reflux/reboil ratio is limited, and
-the liquid hold-up of the column section(s) is significant and must be taken into consideration.

For real industrial operating conditions we have to make rigorous simulation calculations.

The goals of the paper are
-to verify the conclusions of the feasibility studies,
-to investigate the performance of the feasible configurations,
-to compare the different configurations with rigorous simulation calculations.

The calculation results are presented for the mixtures ethanol (***A***) ï toluene (***B***) (minimum boiling point azeotrope) and water (***A***) ï ethylene-diamine (***B***) (maximum boiling point azeotrope).

VLE CONDITIONS

The y-x equilibrium diagrams and azeotropic data at the different pressures of the mixtures studied are shown in *Fig. 1* and *Table 1*, respectively.

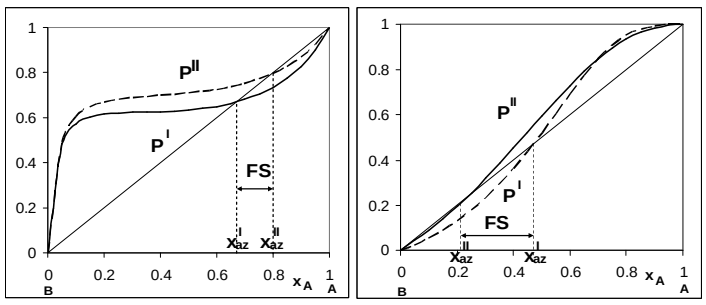

Fig. 1. y-x diagrams of the mixtures
a. ethanol ï toluene (P^I=0.1, P^{II}=1.1 bar)
b. water- EDA (P^I=0.1, P^{II}=8.0 bar)

Mixture	*P* [bar]	x_{az} [mol%]	T_{az} [°C]	$T_{BP,A}$ [°C]	$T_{BP,B}$ [°C]
Ethanol (***A***)-	0.1	67	26.4	29.1	45.3
Toluene (***B***)	1.1	79	78.8	80.4	113.6
Water (***A***)-	0.1	47	62.2	45.8	50.8
EDA (***B***)	8.0	21	199.5	170.5	198.6

Table 1. Data of azeotropes

By varying the pressure the azeotropic compositions are shifted.

RIGOROUS SIMULATION CALCULATIONS

After the feasibility studies we performed rigorous simulation calculations for real operating conditions.

Simulation method

The following simplifying assumptions were applied
- theoretical stages,
- negligible vapour hold-up,
- constant volumetric liquid plate hold-up.

For the calculations we used the CCDCOLUMN professional dynamic flow-sheet simulator of Chemstations.

Simulation results

The following configurations are studied. For the separation of
a. maximum azeotropes: BR, BR-BS, DCBR
b. minimum azeotropes: BS, BR-BS, DCBS
Input data:
N=20, U^{vol}=50 or 25cm^3/plate, U_{ch}=11dm^3
Ethanol ï toluene: R=S=20, x_{ch}=0.71, dP/dt=0.2 bar/min
Water-EDA: R=S=15, x_{ch}= 0.4, dP/dt=1 bar/min
At the start the column is filled up with boiling point liquid feed. The duration of the start-up period (purification without product withdrawal) is 60 min. The whole process is finished
-for the BR, BS and BR-BS: the duration of any production step becomes shorter than 15 min,
-for the DCBR and DCRS: the amount of liquid in the vessel decreases to 2% of the charge.

Batch Rectifier and Batch Stripper

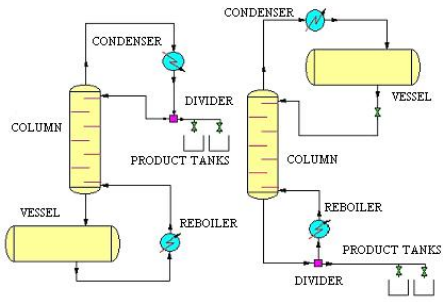

Fig. 2. Scetch of batch rectifier and batch stripper

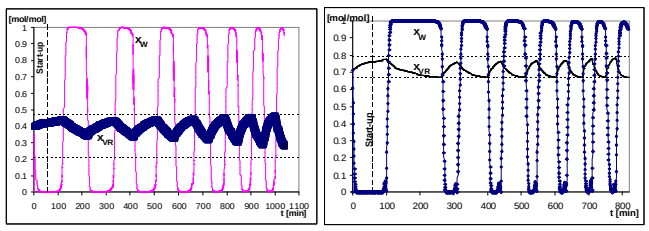

Fig. 3. Evolution of product (x_W) and vessel residue (x_{VR}) compositions for a maximum azeotrope by BR and a minimum azeotrope by BS

With the progress of the process
-the production periods become shorter and shorter,
-the vessel composition varies more and more quickly and in a wider and wider region.
The duration of the periods without product withdrawal (purification, pressure change) is relatively high (*Tables 2-3)*.

Combination of the batch rectifier and stripper

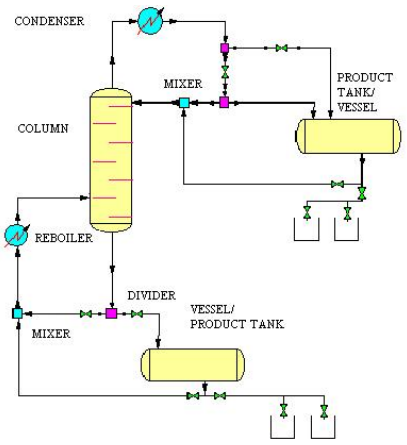

Fig. 4. Scetch of the combination of the batch rectifier and stripper

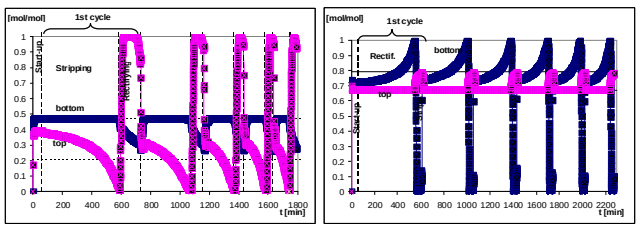

Fig. 5 Evolution of top vapour and bottom liquid compositions for the BR-BS
a. maximum azeotrope *b. minimum azeotrope*

In the start-up period the product takes the azeotropic composition quickly, and keeps it until the end of the 1-st step of the cycle. The vessel liquid reaches high purity by that time and then it is removed from the vessel, which will be the product tank in the 2nd step of the cycle performed at the another pressure. In this tank after a short transient period at the beginning of this 2nd step pure product can be collected. The composition in the vessel (which was product tank in the 1-st step) is approaching to the azeotropic one. The cycles become shorter and shorter.

The duration of the periods without product withdrawal is considerable (*Tables 2-3*).

Double Column Batch Rectifier (DCBR) and Stripper (DCBS)

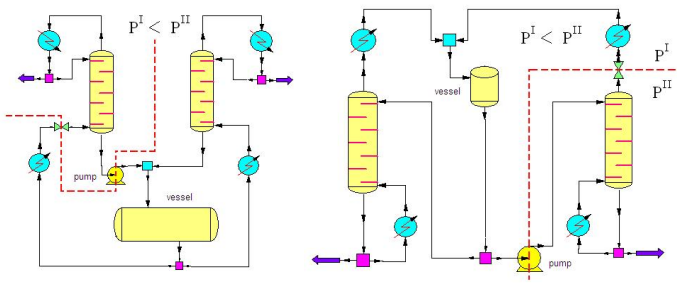

Fig. 6. Scetch of double column batch rectifier and double column batch stripper

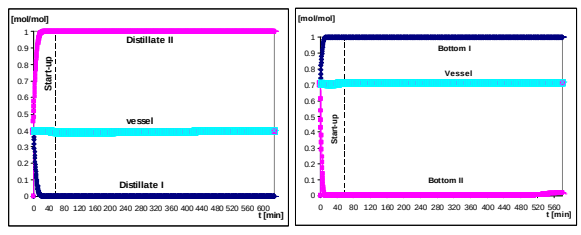

Fig. 7. Evolution of products and vessel residue compositions for a maximum (DCBR) and minimum azeotrope (DCBS)

Both products get pure quickly and purities remain very high for a very long period. The vessel composition remains within a very narrow interval. The highest purities and recoveries are produced by these new double column configurations.

		BR	BR-BS	DCBR
Water-recovery	**%**	**88.7**	**82.7**	**90.2**
EDA-recovery	**%**	**86.2**	**82.0**	**92.6**
Water-purity	**mol %**	**98.99**	**98.02**	**99.99**
EDA-purity	**mol %**	**99.35**	**98.03**	**99.97**
Water energy (SQ/SW_A)	**MJ/mol**	**5.98**	**10.8**	**3.77**
EDA energy (SQ/SW_B)	**MJ/mol**	**4.10**	**7.28**	**2.45**
Total-energy	**MJ**	**495.6**	**836.6**	**316.6**
Total time	**min**	**1039**	**1790**	**687**
Production time	**min**	**598**	**1451**	**627**

Table 2. Results for the mixture Water-EDA

		BS	BR-BS	DCBS
EtOH-recovery	**%**	**80.4**	**63.1**	**92.3**
Toluene-recovery	**%**	**78.0**	**94.5**	**97.8**
EtOH-purity	**mol %**	**99.4**	**98.3**	**99.99**
Toluone-purity	**mol %**	**99.4**	**98.3**	**99.86**
EtOH-energy (SQ/SW_A)	**MJ/mol**	**4.22**	**15.72**	**3.08**
Toluene-energy (SQ/SW_B)	**MJ/mol**	**10.6**	**25.71**	**7.11**
Total-energy	**MJ**	**369.4**	**1080**	**311.5**
Total time	**min**	**877**	**2274**	**680**
Production time	**min**	**464**	**1939**	**620**

Table 3. Results for the mixture Ethanol-Toluene

By thermal coupling of the high pressure condenser with the low pressure reboiler energy can be saved (34.0 (DCBR) and 24.5 % (DCBS) of the total heat duty of the system).

CONCLUSION

The pressure swing distillation of binary mixtures was studied in different batch column configurations by using the CCDCOLUMN dynamic flowsheet simulator. On the basis of the results of feasibility studies we investigated and compared the following configurations for
- minimum azeotropes: batch stripper (BS), double column batch stripper (DCBS),
- maximum azeotropes: batch rectifier (BR), double column batch rectifier (DCBR) and
- for both types of azeotrope: the alternate application of a rectifier and a stripper.

The best results were obtained with the two new configurations (DCBS and DCBR), which do not require pressure change during the process. The rectifier-stripper combination proved to be less efficient than the simplest configurations (BR and BS). We also proved that both column sections of the new DCBS and DCBR configurations can be operated under practically steady state conditions.

REFERENCE

Modla G. and P. Lang, New column configurations for pressure swing batch distillation, I. Feasibility studies, DYCOPS 2007.