CHEMICAL ENGINEERING TRANSACTIONS Volume 25, 2011
Editors Jiří Jaromír Klemeš, Petar Sabev Varbanov, Hon Loong Lam

DOI: 10.3303/CET1125116

Comparison of Closed and Open Operation Modes of Batch Distillation

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Open and non-conventional closed batch column operation modes were compared by rigorous simulation. The configurations studied were the batch rectifier ("two vessel column"), middle- and multi-vessel column ("three and four vessel columns"). For the operation in closed system we studied six different modes differing in the operation of the vessels. We simulated the separation of test mixtures (n-hexane(A)-n-heptane(B), A-B-n-octane(C), A-B-C-n-decane(D)), and compared the recoveries under constant product purities. The effects of the operational parameters were also studied.

1. Introduction

The batch rectifier (BR) is the only widespread batch distillation configuration in the industry operated in open system (with continuous product withdrawal). Middle-vessel column (MVC; Bortolini and Guarise, 1970) consists of two column sections connected through a middle vessel, and can produce three products simultaneously. The generalisation of MVC is the multi-vessel column (MuVC; Wittgens et al., 1996), built up from more column sections and vessels, and is generally operated without product withdrawal. These devices can be operated also in closed mode (without product withdrawal), which may reduce the energy consumption (Skouras and Skogestad, 2004). Two column systems operated in closed mode were suggested by Denes et al. (2009) for heteroazeotropic and Modla (2010) for pressure swing batch distillation.
The aim of this work is to study the competitiveness of closed modes with the open ones. The rigorous simulation calculations are made for a binary (A-B), a ternary (A–B–C) and a quaternary (A–B–C–D) mixture with the dynamic module of the ChemCAD flow-sheet simulator. The recoveries obtained for the same product purities are compared under constant process duration (with the exception of multivessel column).

2. Configurations and operation modes

Simplifying assumptions: theoretical plates, constant liquid and negligible vapour plate hold-ups. For the VLE and enthalpy calculations, the SRK equation of state is applied.

2.1 Batch rectifier

The open and different closed operation modes of BR are compared. The charge is an equimolar mixture of A and B, its volume is 10 dm^3. The prescribed purity of A is 99 mol%. The column operates with a heat duty of 500 W.

Please cite this article as: Hegely L. and Lang P., 2011, Comparison of closed and open operation modes of batch distillation, Chemical Engineering Transactions, 25, 695-700
DOI: 10.3303/CET1125116

2.1.1. Open operation mode

The reflux ratio is constant during the process. The operation is stopped when the A content of the accumulated product decreases to 99 mol%. The duration (Δt) obtained in this way is prescribed for the closed operation modes.

2.1.2. Closed operation modes

The models of the closed modes (Fig. 1a) are very similar; the difference is the presence or lack of the control equipment. The A-rich product is accumulated in the upper vessel.

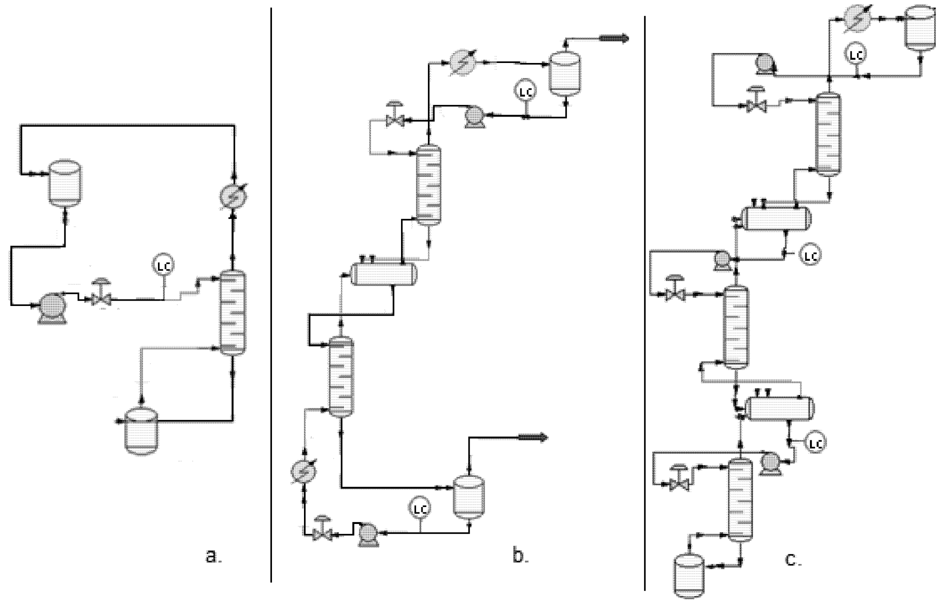

Figure 1: ChemCAD models of closed operation modes with level control a: batch rectifier, b: middle-vessel column, c: multi-vessel column with four vessels

Six different closed modes are presented for the BR (Table 1), which differ in the operation of the upper vessel, that is, in the method of varying the liquid flow rate from this vessel. For closed modes each (further) vessel provides one new degree of freedom (DoF). For closed modes we define R as the ratio of the flow rate of reflux (L) and the rate of product accumulation (V-L).

2.2 Middle-vessel column

The different modes of the MVC are investigated by comparing the recoveries of A and C for the separation of an equimolar mixture (20 dm^3) of A, B and C. The prescribed purities for A and C are 98 mol%. Both column sections have 10 theoretical plates.

2.2.1. Open operation mode

The charge is filled into the middle vessel. The operation begins with total reflux and reboil. The flow rate of the liquid stream leaving the middle vessel is 40 dm^3/h. The reflux and reboil ratios are chosen so that not only the purity of top and bottom products but that of the B-rich product also reaches 98 mol% at the same time. The duration obtained in this way is prescribed for the closed operation modes.

Table :. The closed operation modes of batch rectifier.

Mode	Principle of operation	Additional DoF	Advantage	Disadvantage
Mode 1	Constant volumetric flow rate from the top vessel	Liquid flow rate leaving the vessel	Existence of initial reflux (contrary to Mode 2a)	R is always finite
Mode 2a	Constant level, vessel empty at start	Liquid level	R=∞ after initial period	R=0 initially (accumulation of liquid)
Mode 2b	Constant level, charge is distributed between the vessels	Liquid level (same as the initial level)	R=∞ during the whole operation	Slower dynamics, low purity of initial reflux
Mode 3	Constant flow rate, then constant level (combn. of 1 & 2a)	Flow rate (1st part), liquid level (2nd part)	Faster dynamics at the beginning	Decreased duration of R=∞
Mode 4a	Temperature control, empty vessel at start	Temperature of the 4th plate (from the top)	R≈∞ in the 2nd half of operation	R is finite in the 1st half of operation
Mode 4b	Temperature control, charge is distributed	Temperature of the 4th plate, initial level	The results are virtually the same as those of Mode 4a	

2.2.2. Closed operation modes

The model of the closed modes of the MVC can be seen in Fig. 1b. The upper and lower vessels are operated according to one of the modes presented by the closed modes of batch rectifier. The advantages and drawbacks of the different modes (Table 1) are true for MVC as well, substituting *R* with the reboil ratio for the bottom vessel. The flow rate of the liquid stream leaving the middle vessel is 40 dm^3/h. By Modes 4a and 4b the temperatures of the third (upper column) and the eighth plate (lower one) are controlled. The operation mode applied by Skouras and Skogestad (2004) is also studied. This mode is similar to Mode 4b, but the control is applied to the upper and middle vessels. The temperatures of the middle (fifth) stage of each column sections are controlled, the set-points are the averages of the boiling points of the two components separated in this section. At the start, 94 % of the charge is filled into the bottom, 5 % to the middle, 1 % to the top vessel.

2.3 Multivessel column

The recoveries of A, B, C and D are compared for four closed modes (2a, 2b, 4a and 4b) of MuVC (Fig. 1c). The charge (31.42 dm^3) is equimolar, the purity requirements are 96 mol% for each product. The configuration consists of four vessels, and three column sections, each of them has 8 trays. The hold-up is 40 cm^3/plate. By Modes 4a and b, the temperature of the third plate of each section is controlled. For Mode 4b, the initial liquid level is 0.25 m (7.85 dm^3) in every vessel.

3. Results

The recoveries obtained with the open (only BR and MVC) and different closed modes are compared for the same product qualities. In the case of closed modes the value of at least one operation parameter has to be adjusted in order to maximise the recovery. The PI controllers for the closed modes (except Mode 1) are tuned by the Ziegler-Nichols method. In a few cases, even exponential filters have to be applied. The results of Mode 4b are only presented for MuVC, as the division of charge doesn't have significant effect on the recoveries in the cases of BR and MVC, by our experiences.

Table 2: The effect of N and the hold-up on the recoveries of A.

N	8	10			12
Hold-up (cm^3/p.)	0	0	50	100	0
Open	92.2%	93.3%	95.2%	94.4%	93.6%
Mode 1	88.7%	92.0%	91.7%	89.8%	92.5%
Mode 2a	93.0%	97.1%	92.8%	88.4%	97.9%
Mode 2b	93.9%	97.7%	93.3%	88.9%	98.5%
Mode 3	93.3%	97.1%	92.8%	88.4%	98.0%
Mode 4a	94.1%	97.4%	93.2%	88.8%	98.0%

3.1 Batch rectifier

The effects of three operational parameters on the recovery are studied (Table 2). The reflux ratio of the open mode (R_{open}) and the number of theoretical plates (N) have only slight effects, while the influence of the plate hold-up is very significant. In case of negligible hold-up the closed operation modes (except Mode 1) give better results than the open one. However, when the hold-up is greater, the open operation mode provides better recoveries (Fig. 2a). The advantage of the closed operation modes over the open one is also affected by R_{open}, (that is Δt) and N, though to a smaller extent. The difference increases with increasing N, and decreasing R_{open}.

Mode 1 proved to be always worse than the open mode, and generally worse than the other closed modes. The order of the other closed operation modes (with decreasing recoveries): 2b, 4a, 3, 2a. Mode 2b gave the best recovery with the exception of one case (R_{open}=7), in which it is preceded by Mode 4a.

3.2 Middle-vessel column

We performed the calculation for negligible and 40 cm^3/plate hold-up (4 % of the charge), as well. The recoveries for 40 cm^3/plate hold-up are presented in Table 3, along with the recovery and purity of B. Unlike the BR, the open mode always proved to be better than the closed ones (Fig. 2b). The order of the operation modes with respect to the recoveries is different not only for zero and non-zero hold-ups, but also for A and C. While Mode 2b is the best closed operation mode of the BR, it is not very favourable in the case of the MVC. In case of negligible hold-up, Modes 3 or 4a, in the case of 40

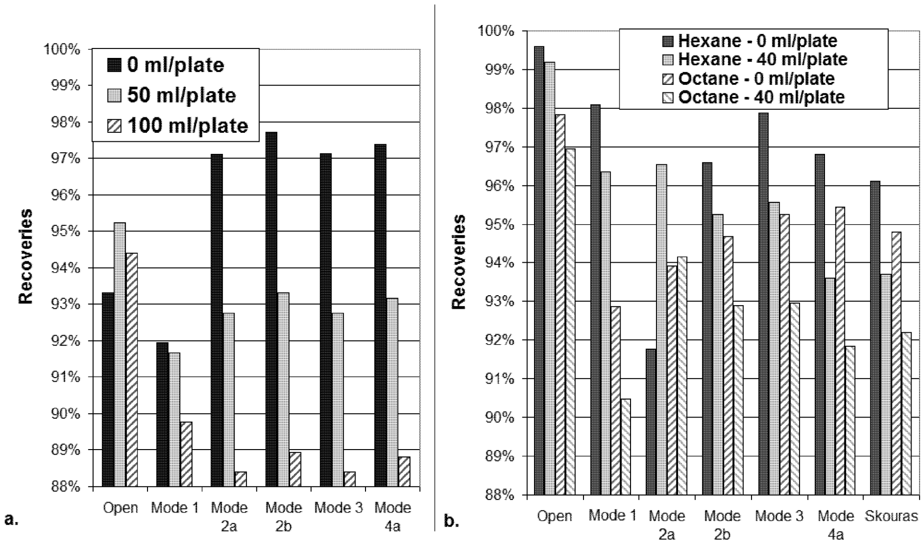

Figure 2:The recoveries at different levels of hold-up (a: BR, N=10, R_{open}=9; b: MVC)

Table 3: The calculated results of MVC (hold-up: 40 cm³/plate).

Hold-up: 40 cm³/p.	Recovery (%)			Purity of B (mol%)
	Hexane (A)	Heptane (B)	Octane (C)	
Open	99.2	73.14	96.94	98.03
Mode 1	96.34	85.63	90.48	94.37
Mode 2a	96.55	84.03	94.15	96.63
Mode 2b	95.25	85.39	92.88	96.66
Mode 3	95.56	86.09	92.96	96.75
Mode 4a	93.61	80.94	91.83	96.69
Skouras	93.7	83.4	92.2	96.62

Table 4: The calculated results of multi-vessel column

	Δt (min)		A	B	C	D	Average
Mode 2a	16.55	Recovery (%)	94.77	80.57	82.60	97.62	**88.89**
		Purity (%)	*96.01*	*96.01*	*96.00*	*96.17*	*96.05*
Mode 2b	25.85	Recovery (%)	95.38	80.16	82.60	98.63	**89.19**
		Purity (%)	*96.07*	*96.06*	*96.00*	*96.07*	*96.05*
Mode 4a	18.25	Recovery (%)	95.38	79.76	83.82	96.19	**88.79**
		Purity (%)	*96.01*	*96.01*	*96.00*	*96.98*	*96.25*
Mode 4b	22.75	Recovery (%)	95.59	79.55	84.02	97.21	**89.09**
		Purity (%)	*96.01*	*96.00*	*96.00*	*97.13*	*96.29*

ml/plate hold-up, Mode 2a and 3 can be suggested. The operation mode of Skouras andSkogestad (2004) gives very similar results to those of Mode 4a, though the purity of A is slightly higher (98.4 mol%).

3.3 Multivessel column

The average recoveries (Table 4) of the different modes are similar. However the energy consumption (proportional to Δt) is the lowest by Mode 2a. The division of charge increases Δt, while the increasement of the average recovery is only slight.

4. Conclusion

The open and six different closed operation modes of batch rectifier (BR) and middle-vessel column (MVC) were studied by rigorous dynamic simulation with ChemCAD. Four closed modes (Modes 2a, 2b, 4a, 4b) of the multivessel column (MuVC) were also investigated. The closed modes differ from each other in the operation of the vessels.

For the batch rectifier closed operation provided better recoveries in case of negligible liquid hold-up. Modes 2b (level control with initially filled up top vessel) and 4a (composition control with initially empty top vessel) proved to be the best closed modes. The decrease of the process duration and increase of number of stages increased the advantage of closed modes. For higher hold-ups, the open operation mode gave the highest recovery.

For the middle-vessel column the open operation mode proved to be better than the closed ones in every case. It was not possible to choose the best closed mode, as the order of the closed modes with respect to the recoveries is not the same for the two products or for the two different hold-ups. For negligible liquid hold-up, Modes 4a or 3 (constant flow rate then level control), for higher hold-ups Mode 2a (level control with initially empty top and bottom vessels) can be recommended.

For the multivessel column the energy consumption of Mode 2a was the lowest, while the recoveries were similar for all modes. The divison of the charge had adverse effect on energy consumption (proportional to the process duration).

Acknowledgement

This work was supported by the OTKA project No.: T-049184 and by the New Hungary Development Plan Project ID: TÁMOP-4.2.1/B-09/1/KMR-2010-0002.

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