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Comprehensive Process Investigation Methodology for Energy-Integrated Distillation

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Abstract

A comprehensive process investigation/design methodology is presented that combines economic, control, and environmental features. The methodology is presented on the case study of energy integrated distillation columns separating ternary hydrocarbon mixtures of different ease of separations. The economic features involve capital and operating costs; the controllability investigations are based on the evaluation of frequency dependent features and dynamic simulations; the environmental evaluation counts for the CO_2 emissions. The results show that the heat integrated scheme is practically the best selection from every point of view.

Keywords: distillation, energy integration, controllability, distillation control, dynamic simulation

1. Introduction

In the course of process synthesis the evaluation of the economic and controllability features of the design alternatives must take place simultaneously. Nowadays, due to increasing environmental regulations the emissions of the alternatives should be also considered. The most frequently studied process design task is the design of separation based on distillation. Due to its high energy consumption of such separation units, energy integrated alternatives are favoured such as heat integration, heat pumping or thermocoupling. Heat integration is an important method for energy conservation, demonstrated by authors Annakou and Mizsey (1996). They have studied heat-integrated schemes and thermally coupled distillation systems by rigorous modelling and compared them to conventional schemes. They have found that the heat-integrated schemes are always more economic than the best conventional scheme. However, it is known that energy integration involves cost savings, these integrated distillation systems have not been widely used in industry due to the control difficulties. Engelien and Skogestad (2004) selected appropriate control variables for sloppy distillation system with forward heat integration. This work contains dynamic simulation results, which show that the distillation structure is controllable, but the system is quite sensitive to disturbances. Segovia-Hernandez et al. (2005) have analyzed the dynamic properties of alternative sequences of the Petlyuk column and they have found that the theoretical controllability properties of the Petlyuk column are not improved by all of the alternative sequences. None of the works, however, provide a comprehensive investigation of energy-integrated distillation systems referring to all economic features, controllability, dynamic behaviour, and environmental impact.

2. Systems studied

Heat-integrated distillation scheme with backward heat integration (DQB). In the case of the separation of ternary mixtures, the heat-integrated distillation system consists of two columns. The base idea of this distillation system is to use the overhead vapour from the second high-pressure column to provide heat to the first low-pressure column (Figure 1.).

Fully thermally coupled distillation column (FTCDC). Fully thermally coupled distillation column is also called Petlyuk column consists of a prefractionator and a main column. The required heat amount for the separation is provided through direct contact of the material flows (Figure 2).

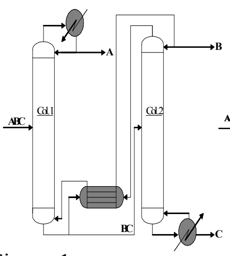

Figure 1
DQB

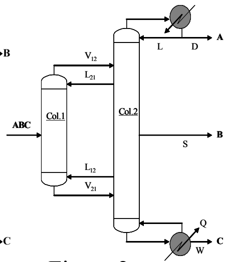

Figure 2
FTCDC

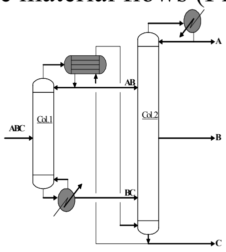

Figure 3
SQF

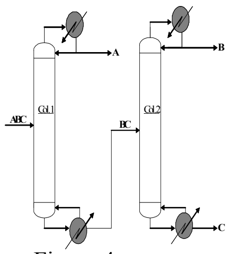

Figure 4
Conventional Direct

Sloppy distillation system with forward heat integration (SQF). This distillation system basically is a heat-integrated sequence, but in the prefractionator sloppy separation takes place. (Figure 3.). The forward scheme

was selected in this work because previous studies (Emtir et al., 2003) have shown that it is easier to control than the backward integration.
Conventional direct distillation scheme is used for comparison. It consists of two simple distillation columns connected in such a way that bottom product of the first column is the feed of the second column. (Figure 4).

3. Case studies

Investigating economic features of the distillation systems three different ternary mixtures are studied and three product purities are expected (Table 1-2). Feed flow rate is 100 kmol/hr and its composition is always equimolar. The chosen ternary mixtures have different ease of separation that can be characterized by the separation index (SI):

$$SI = \alpha_{AB} / \alpha_{BC} \tag{1}$$

In mixture 1 A/B separation is almost as difficult as B/C separation (SI~1). In mixture 2 A/B separation is more difficult than B/C separation (SI<1). In mixture 3 B/C separation is more difficult than A/B separation (SI>1). Controllability study and the dynamic simulations are carried out for mixture 1, pentane-hexane-heptane and the required product purity is 95%.

Table 1 Ternary mixtures studied

Case	Mixture	α_A	α_A	α_A	β	SI
1	pentane-hexane-heptane	7.38	2.67	2.67	0.26	1.03
2	isopentane-pentane-hexane	3.62	2.78	1.3	0.68	0.47
3	butane-isopentane-pentane	2.95	1.3	2.26	0.154	1.74

Table 2 Expected product purities

Case	Product Purities (%)
1	99
2	95
3	90

4. Economic Study

Four distillation structures (Figures 1-4) are investigated. Optimal operating conditions are determined for these distillation structures by rigorous tools. Investigating economic features of the distillation systems three different ternary mixtures are studied and three product purities are selected (Table 1-2). Results of the economic study are shown on Figures 5-7. Figure 5 shows the Total Annual Cost (TAC) vs. Separation Index (SI) when the required product purity is 90%. In this case the most economic distillation structure is the heat-integrated distillation scheme with backward heat integration (DQB) followed by the sloppy distillation system with forward heat integration (SQF). Fully thermally coupled distillation columns show savings compared to the conventional direct distillation scheme which is the most expensive distillation structure. If the required product purity is 95% (Figure 6) total annual cost of each distillation structure increases and the most economic distillation structure is SQF but only in case of mixture with SI=0.47. The results are similar also in case of 99% product purity (Figure 7). Although the SQF is not the most economic structure in every case, but it is not as sensible to the increase of product purity as other structures. Economic study demonstrates that the studied distillation schemes run with the lowest costs when the ease of separation is balanced (SI=1). The heat-integrated systems are the most economic arrangements and always better than FTCDC.

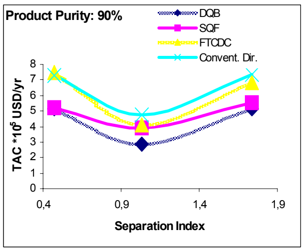

Figure 5

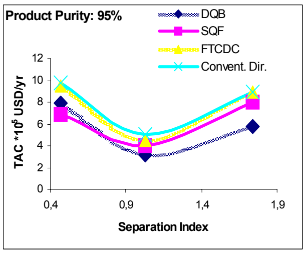

Figure 6

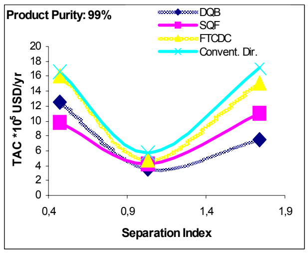

Figure 7

5. Controllability study and dynamic behaviour

The aim of the controllability study is to predict the most promising control structure of the investigated distillation schemes. First, the controlled and manipulated variables are defined for each separation system and the possible pairings of these variables. In this work composition control is proposed to realize. The operating conditions selected for controllability study are: mixture 1 (pentane- hexane- heptane) with equimolar feed composition and 95% product purity. Transfer function matrices (G) are calculated using the CDI interface of the Aspen Dynamics. These transfer function matrices are subjected to singular value decomposition (SVD). Measures used to quantify the degree of directionality and the level of interactions is the condition number (CN), minimal singular value also named Morari resiliency index (MRI) and RGA-number (RGA no). These parameters are used to compare the controllability properties of the distillation schemes. Control structures with the best parameters are tested with closed-loop simulations in time domain. Controlled and manipulated variables define for each distillation structure a 3×3 multivariable system. The chosen manipulated variables for each column are: L – reflux rate (kmol/hr); R- reflux ratio; D – distillate flow rate (kmol/hr); B – bottom product rate (kmol/hr); Q - heat duty of the reboiler (kW). Possible control structures which have CN larger than 10 or MRI less then 10^{-4} are excluded. Based on the controllability results the most promising control structure is selected for each distillation structure which is subject to dynamic simulation. SVD parameters indicate in case of conventional direct distillation scheme and DQB distillation scheme that the possible manipulated variables should be DLB (Figure 8). For FTCDC the proposed control structure based on SVD is LSQ. Suggested control structure for SQF is LSB. The selected control structures are analyzed in time domain in order to decide which controlled

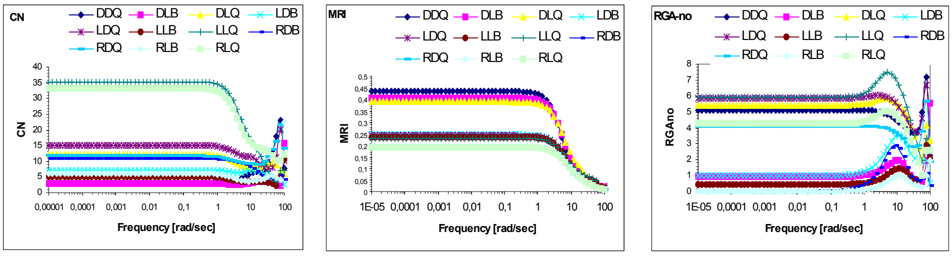

Figure 8 Controllability parameters: CN, MRI, RGA no of DQB scheme

distillation system has better features. In order to study dynamic behaviour of controlled distillation systems feed composition disturbance is used to test the control loop responses. The control loops are detuned when strong interactions are observed. The biggest log modulus tuning. (BLT) method (Luyben, 1986) is used for detuning. Closed loop dynamic simulations show that the heat-integrated distillation scheme is the fastest system and also has the lowest integral absolute error in case of composition control (Table 3).

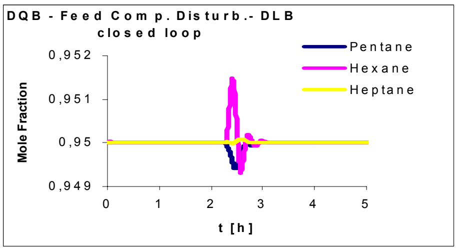

Figure 9
DQB controlled by LSQ control structure

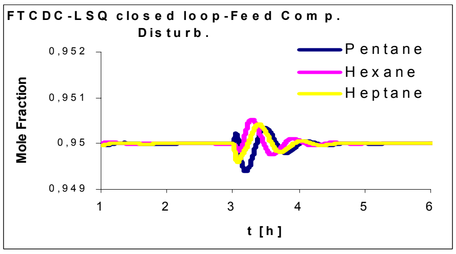

Figure 10
FTCDC controlled by LSQ control structure

Table 3 Results of closed loop dynamic simulation for 1% feed composition disturbance

Feed Comp. Disturb. 1%	Convent. Dir. D-L-B Control struct.		DQB D-L-B Control struct.		FTCDC L-S-Q Control struct.		SQF L-S-B Control struct.	
	IAE 10^{-4}	Settling Time [h]	IAE 10^{-4}	Settling Time [h]	IAE 10^{-4}	Settling Time [h]	IAE 10^{-4}	Settling Time [h]
x_A	3.6	1	1.3	0.5	9	1.6	6.3	1.5
x_B	15	2.6	2.7	0.8	3	2.7	4.3	1.4
x_C	4.8	1.6	0.2	0.4	5	1.5	12	1.5

6. Environmental impact assessment

In the last step of the comprehensive investigation, the environmental impact is estimated. Environmental emission can be assumed to be proportional with the energy consumption of the design alternatives. The energy requirements of the different distillation systems is calculated. The CO_2 emissions are estimated assuming natural gas as heat source and the type of the boiler is: natural gas boiler atmospheric burner low NO_x S [4]. Results show that the CO_2 emission is the lowest in case of heat-integrated distillation schemes including DQB and SQF (Figure 12).

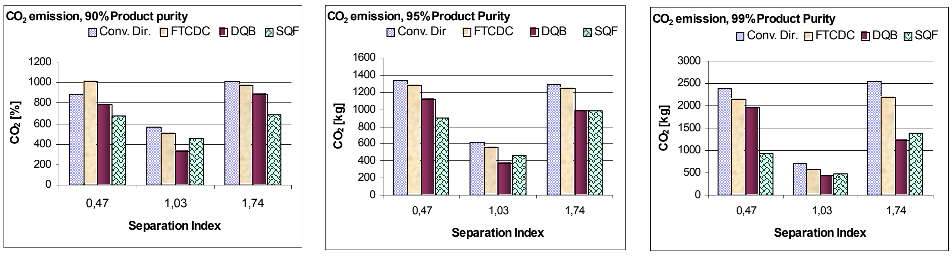

Figure 11 CO_2 emissions in case of 90%, 95%, 99% product purities

7. Conclusions

The comprehensive process investigation methodology, demonstrated on energy-integrated distillation, helps to evaluate process alternatives from a complex point of view: economic, controllability, and environmental impact aspects are simultaneously considered. Economic study shows that the heat-integrated distillation structures have the best economic features. The FTCDC shows energy savings compared to the conventional sequence. Controllability study predicts the suitable control structure. SVD parameters show the system's resilience and the interactions between control loops. Due to the interactions, FTCDC and SQF schemes have worse control features than DQB which is also demonstrated with dynamic closed loop simulations.

In our example the heat-integrated distillation scheme shows the best performance, practically in every issue.

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