

Economic and Controllability Investigation and Comparison of Energy-Integrated Distillation Schemes

M. Emtir, P. Mizsey, E. Rev, and Z. Fonyo

Department of Chemical Engineering, Budapest University of Technology and Economics, H-1521 Budapest, Hungary

Five different energy-integrated distillation schemes: two direct sequences with forward or backward heat integration (**DQF**, **DQB**), the Petlyuk or dividing wall system (**SP**), and two sloppy separation sequences with forward or backward heat integration (**SQF**, **SQB**) are investigated for the separation of a ternary mixture from economic and controllability points of view and compared to the non-integrated conventional direct separation scheme.

The economic study shows that the optimal **DQB** has the highest total annual cost (TAC) saving: 37%. **SQF** and **SQB** have 34% and 33% TAC savings, respectively. The controllability analysis, based on steady state indices, shows that the control loops of **DQF** and **DQB** have less interactions than in the case of the other energy-integrated schemes studied. The dynamic investigations also prove that **DQF** and **DQB** show similar controllability features than the non-integrated conventional scheme. Although the **SQF** and **SQB** have good economic features but their controllability features, especially the ones of **SQB**, are significantly worse than those of **DQF** and **DQB**. Therefore the controllability features should play a significant role at the selection of the energy-integrated distillation schemes.

Keywords:

Energy-integrated distillation scheme, economic optimisation, controllability study

Introduction

In chemical and petrochemical industry distillation units are the most widely used separation technique for fluid mixtures. The main disadvantage of the distillation is its high-energy requirement. Several techniques are used to overcome this problem like integration of the distillation column with the overall processes which can give significant energy saving, e.g. Smith and Linnhoff¹, Mizsey and Fonyo² but these kinds of improvements can be limited. Significant energy savings can be reached by the use of complex distillation arrangements such as side-stripper, side-rectifier, fully thermally coupled distillation column (Petlyuk column), the (external) energy integration (also known as heat-integrated distillation system) and the heat pumping techniques.

Theoretical studies, e.g. Petlyuk *et al.*³, Stupin, Lockhardt⁴, Fonyo *et al.*⁵, Stichlmair, Stemmer⁶, Annakou, Mizsey⁷, Dunneber, Pantelides⁸, Emtir *et al.*⁹, have shown that the thermally coupled column configurations are capable of achieving typically 28–33% of energy savings compared with the best conventional scheme. In addition, the coupling configuration can also be achieved with the so-called dividing wall column, e.g. Wright,¹⁰ Kaibel.¹¹ With this arrangement reduction in capital

cost can be expected. However, the industry has been reluctant to use the Petlyuk configuration and this can be attributed to its limited capability of flexible operation and the fear of control problems.

Annakou and Mizsey⁷ have studied rigorously the fully thermally coupled distillation column or the Petlyuk (or dividing wall) column configuration and the heat integrated scheme for ternary mixture separation. They have recommended a design procedure for the Petlyuk configuration. They have also found that the Petlyuk column is in several cases economically better than the conventional scheme but it is not competitive with heat integrated schemes, except for mixtures of high middle component concentration and for cases where the A/B split is more difficult than B/C and separation is not sharp (90 and 95m %).

Mizsey *et al.*¹² have supported the previous work with controllability study and found that conventional heat-integrated schemes have less interactions compared to Petlyuk column by measuring steady state control indices. The dynamic behaviour shows longer settling times and higher overshoots for the Petlyuk column compared to conventional heat-integrated schemes, detuning is necessary due to strong interaction between its control loops.

Hernandez and Jimenez¹³ have carried out a comparison between energy requirement and con-

Table 1 – Case study: Feed and product specification

Streams:		Feed		Ethanol		n-Propanol		n-Butanol	
Components	α_1	kmol/hr	X	kmol/hr	X	kmol/hr	X	kmol/hr	X
Ethanol (A)	4.7	33.333	0.333	33.168	0.99	0.165	0.005	33.168	0.00
n-propanol (B)	2.3	33.333	0.333	0.335	0.01	32.66	0.990	0.335	0.01
n-butanol (C)	1	33.333	0.333	0.000	0.00	0.165	0.005	0.000	0.99
Total	---	100	1.000	33.503	1.00	32.99	1.000	33.503	1.00

trollability properties for three complex columns including the Petlyuk column. They have found that the schemes with side columns compete economically with the Petlyuk column only for mixtures of low intermediate composition and when B/C split is harder than A/B separation. Schemes with side columns show better dynamic properties than the Petlyuk column, and the amount of middle component has no effect on the control properties.

Bildea and Dimian¹⁴ have studied the relation between design and control of forward and backward heat integration of sloppy separation sequences. They have ideal mixture and have not compared their results with other energy-integrated or non-integrated separation schemes. They have found that the different sloppy heat integrated schemes are quite similar with respect to energy consumption but very different with respect to dynamic behaviour. The forward heat integration alternative is much easier to control than the backward one.

Jimenez et. al.,¹⁵ have compared the controllability properties of thermally coupled distillation schemes with the conventional schemes and their results indicate that the energy-integrated schemes exhibit better control properties than the conventional schemes, and the Petlyuk column shows limited and unstable controllability results.

In this work the comparative design of energy-integrated distillation schemes is carried out and investigated. Since the controllability investigation must be the integral part of the process design, this comparative design includes the economic optimisation of the schemes and the controllability investigation of the optimised schemes. For the final selection both the economic performance and the controllability of the schemes should be taken account. Therefore, firstly the schemes are optimised. The objective function is the total annual cost (TAC). Secondly, the controllability features of the optimised schemes are investigated by determining their steady state control indices, and later on carrying out open loop and closed-loop dynamic simulations for feed rate and composition disturbance.

A case study

For the case study the separation of a ternary mixture of (ethanol – n-propanol – n-butanol) is selected and studied. Feed and product specifications are given in Table 1; product purity of 99m % for the three components is demanded with equal distribution of the impurities in B product stream. Throughout this work, A, B, and C denote the light, intermediate, and heavy components, respectively.

HYSYS flowsheet simulator is used for steady-state and dynamic simulation with the following assumptions:

- UNIQUAC thermodynamic property set is used,
- feed and products are saturated liquids at the actual column pressure,
- pressure drop across distillation columns and heat exchangers are ignored,
- pumping is not considered in cost calculations,
- maximum internal flows are at 65–70 % of the flooding,
- exchange minimum approach temperature (T_{EMA}) in heat exchangers is always constant, 8.5 °C. (This value has been used in several previous works and proved to be adequate, e.g.^{9,16})

In this study the cost for each scheme is assumed to be the sum of utility cost and equipment cost (purchase and installation). Operating costs are assumed to be only utility costs (steam and cooling water). Detailed cost equations are given in Appendix (A1, A2, and A3); utility and cost data are summarised in Table 2.⁹

Table 2 – Utility prices for the case study

Utility	Temperature level (°C)	Price
Low pressure steam	160	17.7 \$/ton
Middle pressure steam	184	21.8 \$/ton
Cooling water	30–45	0.0272 \$/ton
Electricity	-----	0.1 \$/kWh

Energy-integrated distillation schemes

During this comprehensive study first the conventional distillation schemes, the direct (D) and indirect (I) sequences (Figures 1, 2), are studied and considered as base cases for comparison, and secondly five energy-integrated distillation schemes are investigated:

1. direct sequence with forward heat integration **DQF** (Fig. 3),
2. direct sequence with backward heat integration **DQB** (Fig. 4),
3. Petlyuk column (SP) (Fig. 5),
4. sloppy sequence with forward heat integration **SQF** (Fig. 6)
5. sloppy sequence with backward heat integration **SQB** (Fig. 7)

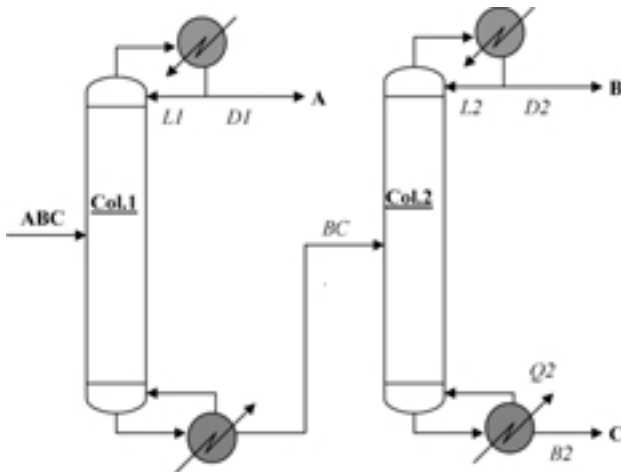


Fig. 1 – Direct sequence (D)

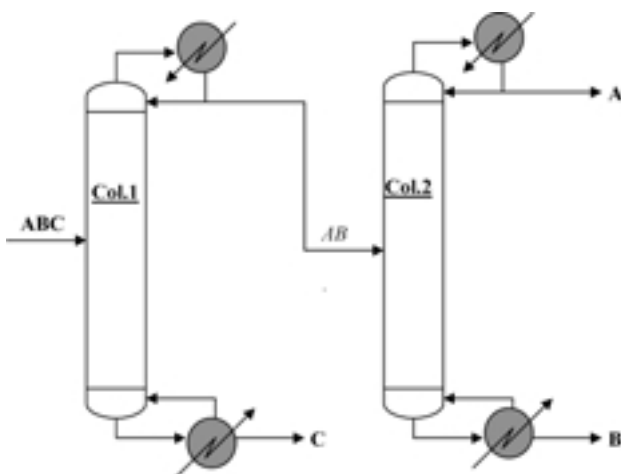


Fig. 2 – Indirect sequence (I)

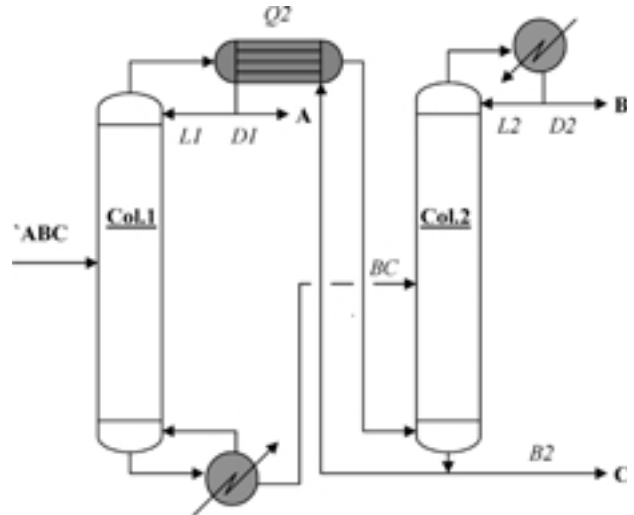


Fig. 3 – Direct sequence with forward heat integration (DQF)

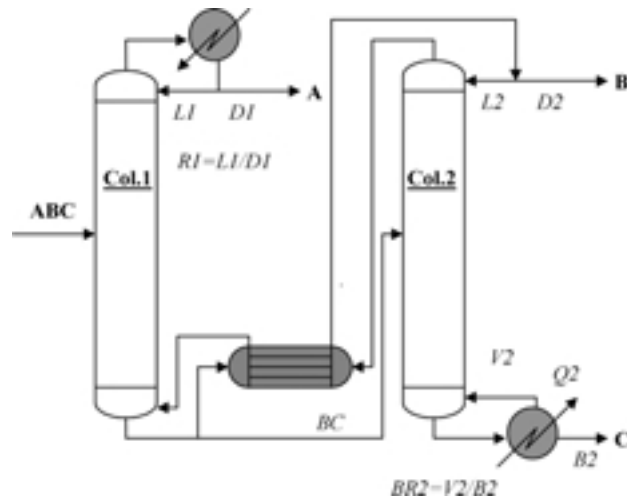


Fig. 4 – Direct sequence with backward heat integration (DQB)

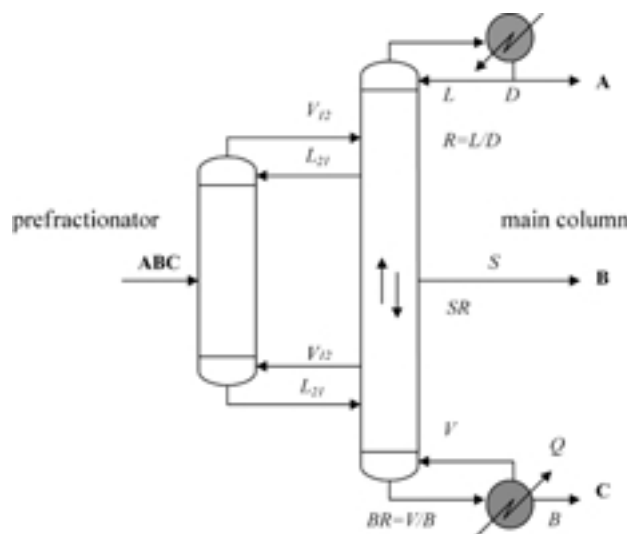


Fig. 5 – Petlyuk system (SP)

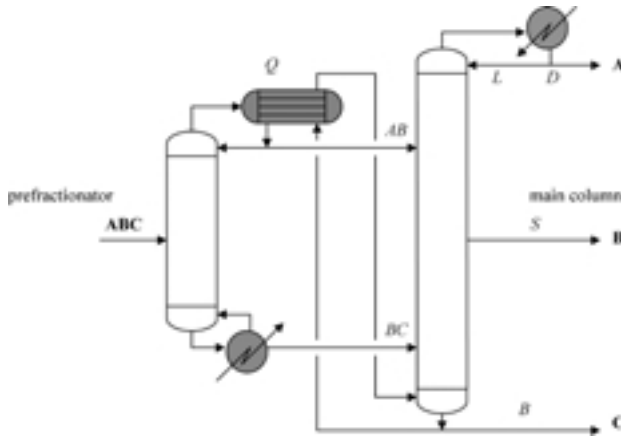


Fig. 6 – Sloppy sequence with forward heat integration (SQF)

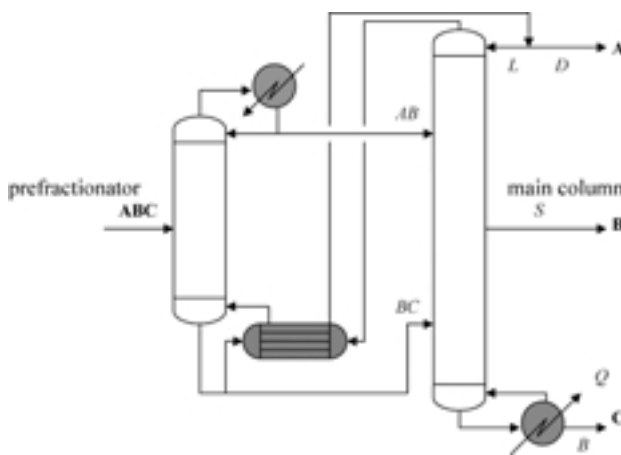


Fig. 7 – Sloppy sequence with backward heat integration (SQB)

Economic study

In the frame of the economic study the optimal parameters of the selected distillation schemes are determined according to the total annual cost (TAC). Interactive and intuitive optimisation methodology is applied for finding the optimal configuration of the different energy-integrated or non-integrated distillation schemes. The optimisation is performed in two hierarchy levels.

1. Column section stage numbers are input data at the lower level. At this level, the continuous variables (column top pressures, reflux ratios, and feed tray locations) are systematically varied over a mesh and the objective values are displayed in matrices of selected variable pairs. The shape of the objective hyper surface over the multidimensional space is intuitively discovered; and the objective and the range around the approximating minimum is rediscovered applying a refined mesh.

2. The section stage numbers are systematically varied in the first level, in a similar fashion. The only difference is that all the possible stage numbers are taken into account, and no refining of the mesh is necessary.

The conventional distillation schemes (D and I) are operated at atmospheric pressure and the optimisation variables are the number of theoretical trays, the reflux ratio, and the feed tray location. The reboiler duty, condenser duty, and the diameter of the columns are also determined. These data are used for costing distillation column and heat exchangers. Since there is no recycled material or energy streams between these columns the optimisation can be performed independently for each column.

Forward heat integration (DQF) can be achieved by raising the pressure of column 1 high enough to make its condenser temperature higher than the bottom temperature of column 2; thus, the first column will boil up the second column. Backward heat integration (DQB) can be achieved by raising the pressure in column 2 high enough to boil up column 1. In almost all cases there is an imbalance between the heat requirements of the two columns; therefore, an auxiliary reboiler or condenser is used. During the interactive and intuitive optimisation of the heat integrated columns the following principles are used:

1. control the operating pressure in the first column or the second column to keep exchange minimum approach temperature at 8.5 °C,
2. keep the lower pressure column at atmospheric pressure,
3. due to energy match between the two columns (heat integration), the optimisation variables are interdependent so the optimisation procedure described above is to be repeated for global optimum.

The sloppy schemes (SQF and SQB) and the Petlyuk column (SP) are also optimised. In these cases column 1 is the prefractionator and column 2 is the so called main column. Their theoretical tray requirements are parameters of the optimisation. Beside the reflux ratio(s) the flows between the prefractionator and the main column and their location are also determined in these cases during the optimisation. In the cases of the SQF and SQB, where heat integration takes also place, the principles mentioned above for heat integration are also followed.

The results of the rigorous optimisation are shown in Table 3 and it can be summarized with respect to TAC savings as follows:

Table 3 – Results of the economic optimisation

Description	D		I		DQF		DQB		SP		SQF		SQB	
	Col.1	Col.2	Col.1	Col.2	Col.1	Col.2	Col.1	Col.2	Prefr	Main col.	Prefr	Main col.	Prefr	Main col.
$T_B(^{\circ}\text{C})$	102.32	117.22	117.19	96.93	153.60	117.21	102.32	134.11	102.37	117.19	150.45	117.24	103.82	158.77
P (kPa)	101.33	101.33	101.33	101.33	511.00	101.33	101.33	178.50	101.33	101.33	451.00	101.33	101.33	367.00
d (m)	0.84	0.82	0.96	0.78	0.76	0.87	0.84	0.85	0.72	0.98	0.65	0.74	0.71	0.71
R	2.25	1.67	0.90	1.87	2.56	2.38	2.25	2.20	0.67	2.99	0.82	1.92	0.67	1.61
η	0.52	0.49	0.46	0.49	0.63	0.49	0.52	0.53	0.51	0.49	0.59	0.48	0.49	0.56
N_A	91	98	93	88	93	55	92	61	87	145	57	147	79	143
N_{TOTAL}	189		181		148		153		232		204		223	
Q_{REB} (kJ/hr)	8.01E+06		8.99E+06		5.19E+06		4.56E+06		5.28E+06		3.91E+06		3.94E+06	
Q_{COND} (kJ/hr)	7.88E+06		8.85E+06		4.78E+06		4.19E+06		5.15E+06		3.78E+06		3.00E+06	
Q_{HX} (kJ/hr)		3.94E+06		4.26E+06			2.89E+06		3.07E+06	
Steam cost (\$/yr)	5.45E+05		6.11E+05		4.52E+05		3.10E+05		3.59E+05		3.41E+05		3.43E+05	
Cooling Water cost (\$/yr)	2.73E+04		3.07E+04		1.66E+04		1.45E+04		1.79E+04		1.31E+04		1.04E+04	
Operating cost (\$/yr)	5.72E+05		6.41E+05		4.69E+05		3.25E+05		3.77E+05		3.54E+05		3.54E+05	
Capital cost (\$/yr)	7.54E+04		7.85E+04		7.80E+04		8.14E+04		8.18E+04		7.62E+04		7.98E+04	
TAC (\$/yr)	6.48E+05		7.20E+05		5.47E+05		4.06E+05		4.59E+05		4.30E+05		4.33E+05	
Capital cost saving (%)	0		-4		-3		-8		-8		-1		-6	
Operating cost saving (%)	0		-12		18		43		34		38		38	
TAC saving (%)	0		-11		16		37		29		34		33	

– the energy-integrated schemes are always more economical than the conventional distillation schemes.

– **DQB** has the maximum TAC saving, 37 %, compared to the other schemes. **DQF** shows the lowest value, 16 %,

– the sloppy schemes show similar savings: 34 % for **SQF** and 33 % for **SQB**,

– Petlyuk column has the highest utility demand compared to other energy-integrated structures and it has only 29 % saving,

– **SQF** and **SQB** have the lowest values of utility demand but because of using middle pressure steam the utility cost will be higher and they become the second ones according to TAC saving classification.

Controllability study

The controllability study is an integral part of the process design. In the practice, the simultaneous investigation is not preferred but during process design the economic optimisation is usually followed

by the controllability study of the optimal structure of each scheme. However, at the final evaluation of the design alternatives the results of both investigation are considered simultaneously to find the best solution.

Steady state analysis

In the investigated schemes the product compositions (\mathbf{X}_A , \mathbf{X}_B , \mathbf{X}_C) are the controlled variables. All the three product compositions are to be controlled at the same time and the proper set of the manipulated variables and the pairing of the controlled and manipulated variables, that is the composition control structures, are determined.

The possible manipulated variables for the direct sequence (**D**), direct sequence with forward heat integration (**DQF**), and direct sequence with backward heat integration (**DQB**) are the following:

- distillate flow rate of column 1 ($D1$),
- reflux flow rate of column 1 ($L1$),
- distillate flow rate of column 2 ($D2$),
- reflux flow rate of column 2 ($L2$),
- bottom flow rate of column 2 ($B2$).

The manipulated variables for the Petlyuk column (**SP**), sloppy sequence with forward heat integration (**SQF**), and sloppy sequence with backward heat integration (**SQB**) are the following:

- heat duty of the main column (Q),
- the side product flow (S),
- the distillate rate of the main column (D),
- the reflux rate of the main column (L).

Ratio control structures are not considered. The possible manipulated variables are also indicated in the Figures of the schemes (Figures 1, 7). The manipulated variables that are not used for the control of the composition of the products are used for the material balance control. The controllability investigations both the steady-state and the dynamic ones are made also with HYSYS.

Firstly, steady state indices are determined for the 3×3 multivariable systems. The following controllability indices are used:^{17,18} the Niederliski index (NI), the Morari resiliency index (MRI), the relative gain array (RGA or λ), and the condition number (CN). The results are shown in Table 4.

The results indicate the following:

- composition control loops of the base case (**D**) and the conventional heat-integrated schemes (**DQF** and **DQB**) show less interactions,

- the steady state control indices of (**D1-L2-B2**) manipulated variables selection for **D**, **DQF**, and **DQB** schemes seem to be better than the set of (**L1-D2-Q2**) and (**L1-D2-B**),

- serious interactions can be expected for the sloppy schemes (**SQF** & **SQB**) and for the Petlyuk column (**SP**) due to poor relative gain array values and also for the other indices,

- in case of **SP**, **SQF**, and **SQB** schemes the selection of (**L-S-B**) set of manipulated variables is better than (**D-S-Q**) set according to the indices.

The results of steady-state control indices are verified by subsequent dynamic simulation, which include the study of open loop and closed-loop dynamic behaviour of the schemes under feed rate and feed composition disturbance.

Dynamic simulation

For the dynamic simulations equimolar feed composition ($\mathbf{X}_A=0.33$, $\mathbf{X}_B=0.33$, $\mathbf{X}_C=0.33$) and feed rate of 100 kmol/h are selected as base case. The schemes are tested for feed flow and feed composition disturbances. Always only one disturbance is allowed. For feed flow is the disturbance 100 to 100.5 kmol/h and for feed composition (mole frac-

Table 4 – Steady state controllability indices for the optimised schemes

Studied schemes (and manipulated variables)	NI	MRI	CN	λ_{11}	λ_{22}	λ_{33}
D -(D1-L2-B2)	1.137	0.099	8.890	1.000	0.880	0.880
D -(L1-D2-Q2)	1.995	0.065	32.113	1.000	0.500	0.500
D -(L1-D2-B2)	1.865	0.234	4.934	0.580	0.540	0.920
DQF -(D1-L2-B2)	1.136	0.024	36.320	1.000	0.880	0.880
DQF -(L1-D2-Q2)	1.890	0.033	21.290	1.000	0.530	0.530
DQF -(L1-D2-B2)	1.678	0.226	5.240	0.586	0.595	1.020
DQB -(D1-L2-B2)	1.093	0.023	39.660	1.000	0.910	0.910
DQB -(L1-D2-Q2)	2.283	0.040	18.110	1.000	0.440	0.440
DQB -(L1-D2-B2)	1.540	0.246	5.040	0.647	0.645	1.000
SP -(D-S-Q)	3.515	0.182	6.890	1.000	0.320	0.280
SP -(L-S-B)	7.438	0.089	14.380	0.130	0.570	0.990
SQF -(D-S-Q)	6.470	0.010	137.400	1.000	0.250	0.150
SQF -(L-S-B)	4.030	0.008	158.100	0.250	0.250	0.998
SQB -(D-S-Q)	5.080	0.038	33.310	0.997	0.470	0.196
SQB -(L-S-B)	1.287	0.022	64.388	0.770	0.827	1.000

tions) (0.33/0.33/0.33) to (0.32/0.34/0.32), respectively.

Open loop dynamic simulation

In open loop dynamic simulation, the schemes are studied without any composition control and the time constants of the different transient behaviours are estimated (Tables 5, 6).

Table 5 – Open loop performance for feed rate disturbance

Studied schemes	Ethanol (X _A)	n-Propanol (X _B)	n-Butanol (X _C)	Average time constant (time unit)
	Time constant (time unit)	Time constant (time unit)	Time constant (time unit)	
D	16	8	3	9
DQF	20	11	2	11
DQB	14	9	6	10
SP	16	5	6	9
SQF	16	3	5	8
SQB	23	13	11	16

Table 6 – Open loop performance for feed composition disturbance

Studied schemes	Ethanol (X _A)	n-Propanol (X _B)	n-Butanol (X _C)	Average time constant (time unit)
	Time constant (time unit)	Time constant (time unit)	Time constant (time unit)	
D	12	10	6	9
DQF	15	5	19	13
DQB	11	13	6	10
SP	14	7	4	8
SQF	14	2	6	7
SQB	36	9	9	18

The results of the open loop dynamic simulations show that **SQB** is the slowest scheme compared to the others and it has the highest time constant (Tables 5 and 6). The rest of the studied schemes have approximately similar time constants. As examples for the transient open-loop dynamic behaviours: the conventional direct separation sequence with backward heat integration (**DQB**) and the Petlyuk column are shown for feed flow rate and feed composition disturbances (Figures 8, 11).

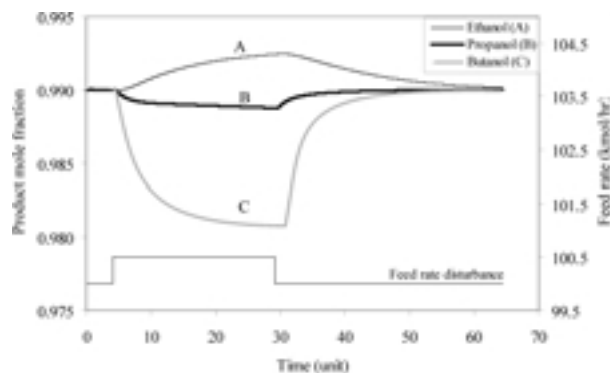


Fig. 8 – The transient behaviour of the Petlyuk column in open loop for feed flow rate disturbance

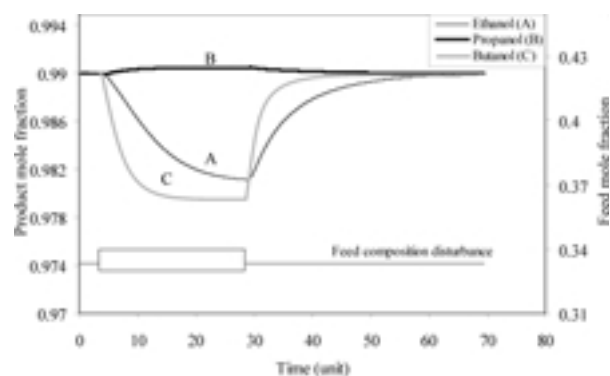


Fig. 9 – The transient behaviour of the Petlyuk column in open loop for feed composition disturbance

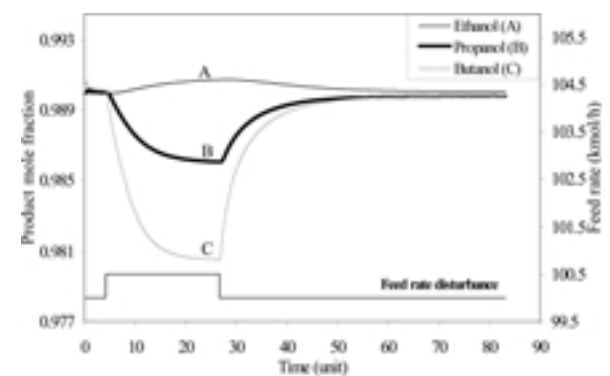


Fig. 10 – Open loop transient behavior of **DQB** scheme for feed rate disturbance

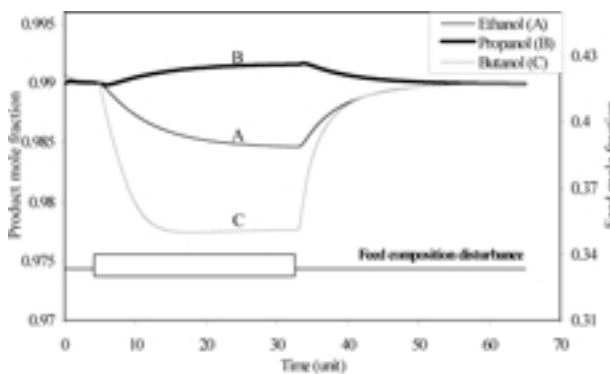


Fig. 11 – Open loop transient behavior of **DQB** scheme for feed composition disturbance

Closed-loop dynamic simulation

Those control structures are selected for closed composition control loop (closed-loop) dynamic simulation that show good steady-state controllability indices. PI controllers are used for the composition control loops and P controllers are used for the material balance control loops (level control). The controller tunings are determined by the Tyreus-Luyben cycling method.¹⁹

Closed-loop simulations are carried out for feed rate and composition disturbances. The settling time, overshoots, and the product of settling time and overshoots (PSO) are determined and compared to characterise the dynamic behaviour of the schemes. PSO values are expected to be proportional to integral square error (ISE) of the control loop. If serious interaction takes place among the control loops, detuning of the controllers is also completed.

The results of the studied schemes are summarised in Tables 7 and 8. They show that the base case (**D**) and the conventional heat-integrated schemes (**DQF**, **DQB**) are the fastest in closed-loop dynamic behaviour by showing lower settling times, overshoots, and PSO values compared to the other investigated schemes (**SP**, **SQF**, and **SQB**). The comparison of the control structures used for

the **D**, **DQF**, and **DQB** schemes shows that the *D1-L2-B2* set of the manipulated variables proves to be faster than the *L1-D2-Q2* and *L1-D2-B2*. The *D-B* structures originally believed to be unworkable but investigated and recommended by Skogestad²⁰ show less favourable performance.

Closed-loop dynamic behaviours of the conventional direct separation sequence with backward heat integration (**DQB**) and the Petlyuk column (**SP**) are shown in Figures 12–15 for feed flow rate and feed composition disturbances. The Petlyuk column shows good dynamic behaviour in closed-loop disturbance compared to sloppy heat-integrated schemes (**SQF** and **SQB**). The *L-S-B* set of manipulated variables (control structure) proves to be faster in closed-loop dynamic simulation than *D-S-Q* set for Petlyuk column and also for sloppy schemes.

Forward energy-integrated schemes show better controllability features than the corresponding backward energy-integrated schemes (**DQF** – **DQB** and **SQF** – **SQB**), and this can be due to stronger interactions that can take place because of the opposite directions of energy and materials flows. A similar phenomenon has been found but only for the sloppy sequences by Bildea, Dimian.¹⁴

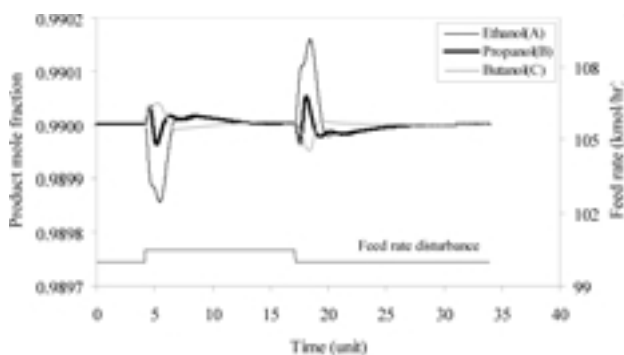
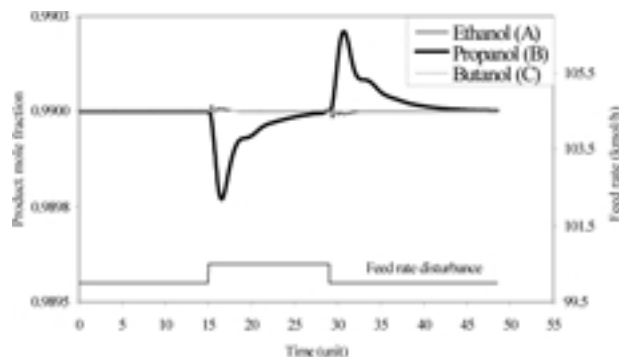
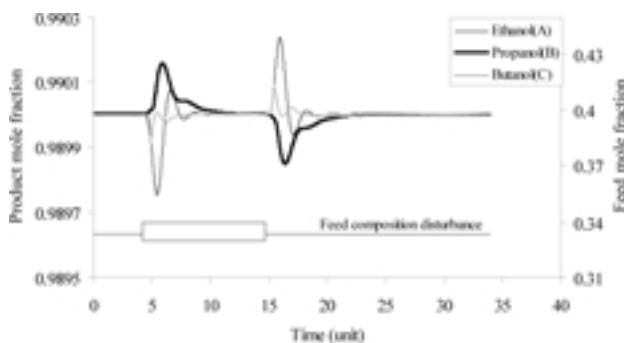
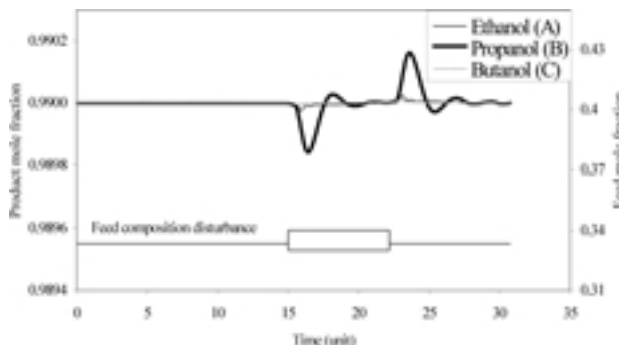
Considering that the **DQF** is economically worse than **DQB** by far it is not preferred to **DQB**

Table 7 – Closed-loop performance for feed rate disturbance

Studied schemes (and manipulated variables)	Ethanol (X_A)		n-Propanol (X_B)		n-Butanol (X_C)		Σ ST	Σ OS	Σ PSO
	Settling time (time unit)	Overshoot (%)	Settling time (time unit)	Overshoot (%)	Settling time (time unit)	Overshoot (%)			
D (<i>D1-L2-B2</i>)	0.960	0.000	7.460	0.010	2.160	0.000	10.580	0.010	0.075
D (<i>L1-D2-B2</i>)	0.500	0.000	21.600	0.010	10.640	0.001	32.740	0.011	0.227
DQF (<i>D1-L2-B2</i>)	0.820	0.000	8.540	0.006	2.260	0.000	11.620	0.006	0.051
DQF (<i>L1-D2-Q2</i>)	0.500	0.000	14.800	0.012	4.800	0.000	20.100	0.012	0.178
DQF (<i>L1-D2-B2</i>)	0.100	0.000	34.100	0.010	2.350	0.002	36.550	0.012	0.346
DQB (<i>D1-L2-B2</i>)	5.800	0.001	13.230	0.023	4.300	0.000	23.330	0.024	0.310
DQB (<i>L1-D2-Q2</i>)	2.650	0.000	22.750	0.033	1.350	0.000	26.750	0.033	0.751
DQB (<i>L1-D2-B2</i>)	6.950	0.000	20.300	0.033	7.000	0.001	34.250	0.034	0.677
SP (<i>L-S-B</i>)	10.810	0.014	11.500	0.004	8.300	0.005	30.610	0.023	0.238
SP (<i>D-S-Q</i>)	13.720	0.006	12.860	0.006	12.860	0.008	39.440	0.020	0.262
SQF (<i>L-S-B</i>)	14.000	0.012	16.500	0.030	10.000	0.015	40.500	0.057	0.813
SQF (<i>D-S-Q</i>)	18.420	0.004	21.890	0.037	19.650	0.001	59.960	0.042	0.903
SQB (<i>L-S-B</i>)	31.520	0.013	31.520	0.011	7.110	0.006	70.150	0.030	0.799
SQB (<i>D-S-Q</i>)	49.000	0.013	52.000	0.015	49.000	0.003	150.000	0.031	1.564

Table 8 – Closed-loop performance for feed composition disturbance

Studied schemes (and manipulated variables)	Ethanol (X_A)		n-Propanol (X_B)		n-Butanol (X_C)		Σ ST	Σ OS	Σ PSO
	Settling time (time unit)	Overshoot (%)	Settling time (time unit)	Overshoot (%)	Settling time (time unit)	Overshoot (%)			
D (<i>D1-L2-B2</i>)	3.460	0.001	8.160	0.005	2.580	0.000	14.200	0.006	0.044
D (<i>L1-D2-B2</i>)	0.500	0.000	12.800	0.020	7.900	0.001	21.200	0.021	0.264
DQF (<i>D1-L2-B2</i>)	2.320	0.000	8.320	0.003	2.520	0.000	13.160	0.003	0.025
DQF (<i>L1-D2-Q2</i>)	1.140	0.000	15.400	0.041	6.800	0.000	23.340	0.041	0.631
DQF (<i>L1-D2-B2</i>)	1.150	0.000	24.300	0.080	6.500	0.001	31.950	0.081	1.951
DQB (<i>D1-L2-B2</i>)	6.040	0.003	7.190	0.016	3.300	0.000	16.530	0.019	0.133
DQB (<i>L1-D2-Q2</i>)	6.550	0.000	29.150	0.130	2.150	0.000	37.850	0.130	3.790
DQB (<i>L1-D2-B2</i>)	8.400	0.001	27.300	0.128	9.140	0.001	44.840	0.130	3.512
SP (<i>L-S-B</i>)	10.300	0.025	10.490	0.016	7.600	0.002	28.390	0.043	0.441
SP (<i>D-S-Q</i>)	14.680	0.016	14.000	0.038	14.000	0.010	42.680	0.064	0.907
SQF (<i>L-S-B</i>)	13.600	0.003	17.000	0.011	11.000	0.003	41.600	0.017	0.261
SQF (<i>D-S-Q</i>)	23.320	0.003	26.970	0.026	18.000	0.001	68.290	0.030	0.789
SQB (<i>L-S-B</i>)	34.200	0.010	48.750	0.060	21.900	0.006	104.850	0.076	3.398
SQB (<i>D-S-Q</i>)	22.500	0.010	62.310	0.070	22.500	0.003	107.310	0.083	4.654

Fig. 12 – The transient behaviour of the Petlyuk column in closed loop for feed flow rate disturbance (*L-S-B* control structure)Fig. 14 – The transient behaviour of the *DQB* scheme in closed loop for feed flow rate disturbance (*D1-L2-B2* control structure)Fig. 13 – The transient behaviour of the Petlyuk column in closed loop for feed composition disturbance (*L-S-B* control structure)Fig. 15 – The transient behaviour of the *DQB* scheme in closed loop for feed composition disturbance (*D1-L2-B2* control structure)

because its controllability features are still acceptable (Figures 14,15). On the contrary, **SQF** and **SQB** show practically similar economic behaviours but since **SQB** shows the worse controllability features among the all, in this case the controllability features make the decision to the favour of **SQF**.

Conclusions

In accordance with the previous comprehensive studies of the energy-integrated distillation schemes,^{7,9,12} in this study also the simplest energy-integrated scheme, the direct separation sequence with backward heat integration shows the highest total annual cost saving. The more complex energy-integrated structures, the sloppy separation sequences with heat integration, and the Petlyuk column show somewhat worse economic features.

The controllability study of the energy-integrated schemes indicates that all the investigated schemes are controllable with decentralized controller structures. In the case of conventional distillation schemes the heat integration doesn't significantly deteriorate the controllability features. On the other hand the more complex structures (Petlyuk column, sloppy heat-integrated-schemes) are more difficult to be controlled due to the serious internal interactions among the control loops. These schemes show worse controllability features than those of the conventional heat-integrated schemes.

In the case of energy integration those alternatives are easier to be controlled where the material flows and the energy flows occur in the same direction. Due to this phenomenon the controllability features become important in the case of the sloppy separation scheme with backward heat integration (**SQB**). During the evaluation of the sloppy heat-integrated schemes the controllability features favour the structure where the material and energy flows occur in the same direction (**SQF**). This controllability differences are, however, not serious in the case of the conventional heat-integrated schemes and the **DQB** scheme can be generally recommended for the case studied. Our results emphasises again the necessity of the simultaneous consideration of the economic and controllability aspects during process design.

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Appendix A1: Sizing and costing of distillation columns

For a given number of theoretical trays, HYSYS simulator calculates column diameter after converging for selected valve tray distillation column with 50.8 mm weir height. Valve trays of Glitsch type are considered. In order to estimate the actual number of trays, overall column efficiency is calculated using simplified equation:²¹

$$\log(E_0) = 1.67 - 0.25 \log(\mu_{org} \alpha_{avg}) + 0.30 \log\left(\frac{L_m}{V_m}\right) + 0.30(h_i) \quad (A.1)$$

$$N_{actual} = \frac{N_{theoretical}}{E_0} \quad (A.2)$$

The height of the column for 0.6 m tray spacing and 6 m disengagement is given by:

$$H = h + 6.0 \quad (A.3)$$

where

$$h = (N_{actual} - 1) \cdot 0.6 \quad (A.4)$$

The costing of distillation columns (carbon steel construction) can be estimated by the following cost equations that are updated with the Marshall & Swift index^{22,23}. (For comparison a single value of $M\&S=1056.8$ is selected, value of the starting year of this research.)

$$\text{Installed cost of column shell,} \quad (A.5)$$

$$\text{\$} = \left(\frac{M\&S}{280}\right) \cdot 2982 \cdot d^{1.066} \cdot H^{0.802}$$

If the design pressure (P) is more than 345 kPa, a correction factor $[1+1.45 \cdot 10^{-4} (P-345)]$ is applied.

$$\text{Installed cost of the column trays,} \quad (A.6)$$

$$\text{\$} = \left(\frac{M\&S}{280}\right) (136.14) d^{1.55} h$$

The total column cost is the sum of the installed cost of column shell and the installed cost of column trays.

Appendix A2: Sizing and costing of heat exchangers

The heat transfer area (A) of heat exchangers was calculated as

$$A = \frac{Q}{U \cdot LMTD}$$

by assuming the following overall heat transfer coefficients (U):

- $U_R = 3400 \text{ kJ/m}^2 \text{ h K}$ for reboilers,
- $U_C = 2800 \text{ kJ/m}^2 \text{ h K}$ for condensers,
- $U_{HX} = 2100 \text{ kJ/m}^2 \text{ h K}$ for liquid/liquid heat exchangers.

The cost of heat exchangers can be correlated as a function of the surface area assuming shell and tube, floating head, and carbon steel construction. The installation prices are updated by the Marshall and Swift index.

$$\text{Installed cost of the heat exchanger,}$$

$$\text{\$} = \left(\frac{M\&S}{280}\right) \cdot 1562 \cdot A^{0.65} \quad (A.8)$$

where: $A = \text{area m}^2$, $18.6 < A < 464.5$ and design pressure up to 1034.2 kPa.

Appendix A3: Annual Capital Cost

The capital cost (purchase plus installation cost) is annualised over a period which is often referred to as plant life time

$$\text{Annual capital cost} = \text{Capital cost/Plant life time} \quad (A.9)$$

$$\text{Total annual cost (TAC)} = \text{Annual operating cost} + \text{Annual capital cost} \quad (A.10)$$

Operating costs were assumed just utility cost (steam and cooling water).

- Plant lifetime = 10 years
- Operating hours = 8000 hrs/year.

Nomenclature

- A – Heat transfer area
- A – Light component
- B – Middle component
- B – Bottom product rate of the main column (kmol/h)
- $B2$ – Bottom product rate of the column 2 (kmol/h)
- C – Heavy component
- Col.1– Column 1
- Col.2– Column 2
- d – Column diameter (m)
- D – Conventional direct sequence
- D – Distillate rate of the main column (kmol/h)
- $D1$ – Distillate rate of column 1 (kmol/h)
- $D2$ – Distillate rate of column 2 (kmol/h)
- DQF – Direct sequence with forward heat integration
- DQB – Direct sequence with backward heat integration
- E_o – Overall plate efficiency
- h_w – Weir height (m)
- h_1 – Liquid height above valve opening (m)
- h – Tray stack height (m)
- H – Column height (m)
- I – Conventional indirect sequence
- ISE – Integral square error
- LP – Low pressure steam
- L_m – Molar liquid flow rate (kmol/h)
- L – Reflux rate of the main column (kmol/h)
- $L1$ – Reflux rate of column 1 (kmol/h)
- $L2$ – Reflux rate of column 2 (kmol/h)
- MP – Middle pressure steam
- $M\&S$ – Marshall and Swift index
- N – Number of trays
- N_A – Actual number of trays
- N_{TOT} – Total actual trays
- OS – Overshoot (%)
- P – Column design pressure (kPa)
- PSO – Product of settling time and overshoot
- Q – Heat duty of main column (kJ/hr)
- Q_{REB} – Heating rate (kJ/h)
- Q_{KOND} – Cooling rate (kJ/h)

Q_{HX} – Duty of the reboiler-condenser of heat integration (kJ/h),

Q_2 – Heat duty of column 2 (kJ/hr)

R – Reflux ratio

S – Side product rate of the main column (kmol/h)

SQB – Sloppy sequence with backward heat integration

SQF – Sloppy sequence with forward heat integration

SP – Thermally coupled sloppy sequence (Petlyuk column)

ST – Settling time (time unit)

T – Temperature

T_B – Bottom temperature

TAC – total annual costs

U_R – Overall heat transfer coefficient for reboilers

U_C – Overall heat transfer coefficient for condensers

U_{HX} – Overall heat transfer coefficient for liquid-liquid heat exchangers

V_m – Molar vapour flow rate (kmol/h)

$X_{A,B,C}$ – Mole fraction of component A or B or C

Greek letters

α – Relative volatility

η – Overall column efficiency

λ – Average latent heat

μ_{avg} – Average viscosity of feed (cP)