Reduction of the Energy Consumption of the Iso-/Normal-Butane Gas Splitting Process by Optimising the Reflux Rate

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In the present study, we set out to examine an energy-reduction method whereby the reflux ratio of the iso-/normal-butane gas-splitting process is optimised. The splitting process used in this study was designed to be capable of handling 4,000 kg/h of mixed butane as a feedstock, to produce 2,600 kg/h of n-butane as the major product. Conventionally, three different feedstock compositions are used in the process. The n-butane concentration of the feedstock can vary from 60 to 98%, depending on the supplier. If a feedstock with a high n-butane concentration is fed into the splitter, the top product would have a high n-butane content, such that it cannot be sold as i-butane. To prevent this, in conventional processing, the operator must manually operate a valve to recirculate the overhead flow to the splitter. As a result, the reflux ratio of the splitter exceeds 90. Although a feedstock with a high n-butane content is fed into the splitter for only 2 h/day, the heat duty of the reboiler and condenser in the splitter increases due to the increased reflux rate. In addition, the amount of gas in the splitter increases due to the unequal mass balance, which imposes an extra load on the splitter. If the process could be modified to satisfy product specifications by minimising the reflux rate and thus reducing the unnecessary heat duty, energy optimisation would be possible. Therefore, to reduce the heat duty, in this study, we considered the use of an additional overhead buffer tank to store the top product, instead of recirculating the product to the splitter. In addition, we defined the following three constraint functions to identify the objective function, thus minimising the heat duty: 1) The concentration of n-butane in the major product is always > 99%; 2) When a feedstock with a high n-butane concentration is used, the n-butane concentration in the overhead flow is > 98.5%; 3) When a feedstock with a low concentration of n-butane is used, the concentration of the i-butane overhead flow is > 75%. As a result, when a feedstock with a high concentration of n-butane was used, the composition of n-butane in the overhead flow was 98.683% and the heat duty reduced to 7,242.017 kW. For a feedstock with a low n-butane concentration, the i-butane concentration of the overhead flow was 88.448% and the heat duty was 1116.469 kW. We assumed that the process would run for 8,000 h/year and that feedstocks with low and high n-butane contents would be fed to the splitter for 22 and 2 h/day, respectively. The reduction in the energy consumption as a result of this optimisation was determined to be 13.015 GW/year, corresponding to a financial saving of $1.124 million/year.

1. Introduction

In Korea, the energy consumed by the industrial sector accounts for 50% of the country's total energy consumption, with 30% being consumed by the chemical industry. Distillation processes are highly energy-intensive processes that account for about 40% of the energy consumed by the chemical industry. In addition, the separation phases of a chemical process consume a very large proportion of the energy used and are responsible for much of the initial equipment investment cost. In a typical chemical process, the separation process accounts for 40–80% of the investment cost, and in a large-scale chemical process, more than 50% of the total operating cost can be attributed to the separation process. In addition, more than 70% of the energy consumed by the separation process is required for the distillation. Therefore, any means of saving energy in the distillation process would be of great significance for reducing the overall energy consumption of the country (Lee et al., 2017).

Iso-butane (i-butane) is obtained from the refining of oil. The uses of i-butane include the production of high-density polyethylene (HDPE) raw materials and i-paraffins (Yeochun NCC, 2017). To control the volatility of road fuels, i-butane is mixed directly with the fuel (Mears and Eastman, 2005). Furthermore, i-butane is used in organic synthesis, refrigerants, aerosol propellants, and synthetic rubbers (Larranaga, Lewis, and Lewis, 2016). Similarly, normal-butane (n-butane) is also obtained from oil refining and is used to produce raw materials for organic synthesis and the production of synthetic rubber and high-octane-number liquid fuels (Lewis, 2007). In addition, n-butane is used in the synthesis of maleic anhydride, ethylene, and similar products, acetic acid and other oxidised products, formic acid, and i-butane (Mears and Eastman, 2000).

The splitting process used in the present study was designed assuming a feedstock supply of 4,000 kg/h of mixed butane, producing 2,600 kg/h of n-butane as the major product and i-butane as a minor product at the top of the splitter (the overhead product). The n-butane concentration of the feedstock was found to vary from 60 to 98% depending on the supplier. Thus, when a feedstock with a high n-butane concentration was fed into the splitter, the overhead product would also contain a large amount of n-butane, preventing its being sold as i-butane. To prevent this, the operator manually operates a valve to recirculate the overhead flow to the splitter. As a result, the distillate flow decreases dramatically and the reflux ratio of the splitter becomes > 90. Although the feedstock with a high n-butane content is fed to the splitter for only a short time, specifically, 2 h/day, the heat duties of the reboiler and condenser in the splitter increase due to the increase in the reflux ratio. In addition, a mass imbalance occurs as a result of gas accumulating in the splitter while the load on the splitter increases. By modifying the process to satisfy the product specifications while minimising the reflux rate to eliminate any unnecessary heat duty, the energy consumption may be optimised. Therefore, we propose the optimisation of this process using the Aspen Plus simulation program to calculate the heat duty and the reduction in the energy consumption.

2. Simulation

2.1 Process model

The process model developed in the present study separated the system into two parts, viz. (i) the heat exchanger between the feedstock and the main product (n-butane) and (ii) two splitters (DA-141 and DA-141A on the left and on the right of the process model, respectively). The feedstock is heated up through the heat exchanger and split into two streams before it enters the splitter. Each splitter contains 78 trays, with the feedstock introduced into tray 35. n-butane is extracted from tray 64, where its concentration is the highest. The bottom and overhead flows are combined and stored in one tank for subsequent sale as i-butane.
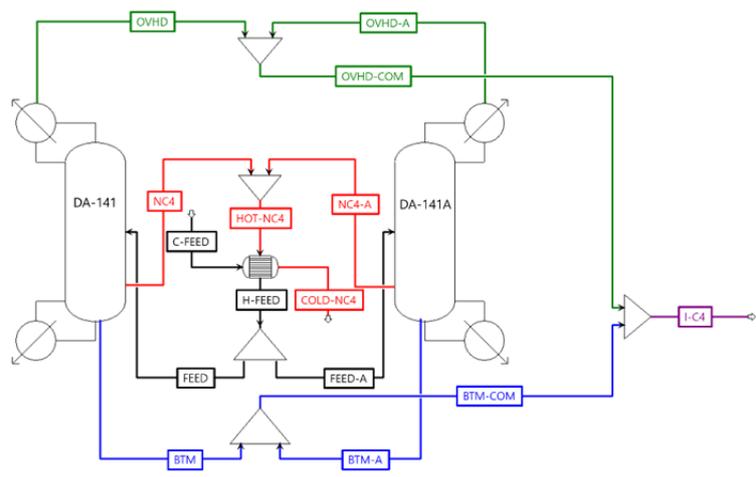
Figure 1. Process flow diagram for the present study (created using Aspen Plus V10)

2.2 Validation of the simulation model

Before attempting any optimisation, we first validated the simulation model, by simulating the target process using the design data. The Peng-Robinson model, a suitable model for the gas phase, was selected as the thermodynamic model, and material properties were chosen. The chosen design data featured an n-butane fraction of 96.7 wt%, because the concentration of n-butane is known to be high and relatively close to that of the target case addressed in the present study. As shown in Table 1, the simulation results closely

approximated the design data, with the slight discrepancy is ascribed to the deviation between the result predicted from the thermodynamic equation and the actual phenomenon. Thus, we concluded that the simulation program is reliable, and therefore conducted our research using the actual operating process data.

Table 1. Simulation model validation by comparing with design specifications

		Main product (side flow)			Minor product (overhead flow)			Bottom product (bottom flow)		
		Design	Simulation	Error	Design	Simulation	Error	Design	Simulation	Error
Propane	kg/h	0.00	0.00	0.00	3.00	3.00	0.00	0.00	0.00	0.00
i-Butane	kg/h	16.90	17.00	0.10	74.00	73.90	−0.10	0.00	0.00	0.00
n-Butane	kg/h	2,917.95	2,917.94	−0.01	12.05	12.05	0.00	9.15	9.11	−0.04
1-Butene	kg/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
i-Butene	kg/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
t-2-Butene	kg/h	3.65	3.67	0.02	0.00	0.01	0.01	0.02	0.01	−0.01
c-2-Butene	kg/h	1.25	1.24	−0.01	0.00	0.00	0.00	0.01	0.01	0.00
n-Pentane	kg/h	0.25	0.20	−0.05	0.00	0.00	0.00	0.30	0.35	0.05
i-Pentane	kg/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	kg/h	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Mass flow	kg/h	2,940.00	2,940.05	0.05	89.05	88.97	−0.08	9.48	9.48	0.00
Temperature	°C	73.0	72.9	−0.15	51	51	0.00	74.0	74.4	0.04
Pressure	kg/cm²G	7.8	7.8	0.00	7.3	7.3	0.00	7.9	7.9	0.00

2.3 Input operating data for simulation

The input values for the simulation were taken from the actual operating data of the process. The required process data must represent a steady state, but the actual process is very dynamic owing to the n-butane concentration of the feedstock. We assumed that any change in the operating data (composition of the feedstock and product) would be insignificant over the course of one hour. Therefore, we assumed a steady state.

Further, we examined two separate cases, which differed according to the n-butane concentration of the feedstock. Henceforth, we will refer to these as the *alpha* and *beta* cases. The n-butane concentration of the feedstock was 70.56% in the alpha case and 90.47% in the beta case. The compositions of the feedstocks also differed between the two cases. The values are listed in Tables 2 and 3.

Table 2. Feed compositions for the alpha and beta cases

Component	Unit	Alpha	Beta
Ethane		0.03	0.00
Propane		1.07	0.00
Propylene		0.00	0.00
i-Butane		27.81	0.35
n-Butane		70.56	98.47
Trans-2-butene		0.08	0.06
1-Butene		0.00	0.06
i-Butene	wt%	0.00	0.06
Cis-2-butene		0.00	0.06
1,3-Butadiene		0.00	0.06
1,2-Butadiene		0.00	0.06
i-Pentane		0.45	0.40
n-Pentane		0.00	0.40
Water		0.00	0.01
Total		100.00	100.00

Table 3. Input data for the alpha and beta cases

Item	Unit	Alpha case			Beta case		
		DA141	DA141A	Total	DA141	DA141A	Total
Feed flow	kg/h	3,732.44	4,012.24	7,744.68	3,710.78	3,986.78	7,697.56
n-Butane product flow	kg/h	2,600.25	2,599.67	5,199.92	2,600.81	2,598.83	5,199.64
Bottom flow	kg/h	79.99	82.00	161.99	80.02	85.75	165.77
Overhead flow	kg/h	1,052.20	1,412.57	2,464.77	1,029.95	1,387.95	2,417.90
Reflux flow	kg/h	19,355.10	18,781.30	38,136.40	21,056.90	20,870.50	41,927.40
Overhead pressure	kg/cm^2	7.30	7.25	–	7.29	7.25	–
Bottom pressure	kg/cm^2	7.86	7.81	–	7.77	7.75	–
Feed temperature before heat exchanger	°C	25.22	25.22	–	25.39	25.39	–
Feed temperature after heat exchanger	°C	44.02	44.02	–	44.02	44.02	–
Reflux temperature	°C	29.94	29.94	–	30.08	30.08	–

2.4 Simulation results

The simulation results for the main flow rates of the process are listed in Table 4. In the alpha case, slight differences in the overhead flow and the temperature of the splitter can be observed due to the problems encountered in the process. In other words, the process data were collected using the distributed control system (DCS) and were recorded at 1-min intervals, i.e. the operating values were recorded as the one-minute average. Consequently, the monitor failed to record data in real time, and the acquired data were incorrect; however, the simulation data was calculated as steady-state simulation. In the beta case, a large difference is observed for overhead flow because in the actual process, the operator manually controls all the variables based on his/her experience, with the overhead stream being forcibly refluxed by adjusting the valve to significantly increase the reflux rate in the splitter. Since this process is not economical, we propose a modified version to reduce unnecessary energy consumption and use Aspen Plus to optimise the process and thus improve the product yield and purity.

Table 4. Simulation results for the alpha and beta cases

Item	Unit	Alpha case			Beta case		
		Operating	Simulation	Error	Operating	Simulation	Error
Feed flow	kg/h	7,744.68	7,744.68	0.00%	7,697.56	7,697.56	0.00%
n-butane flow	kg/h	5,199.92	5,199.92	0.00%	5,199.64	5,199.64	0.00%
Bottom flow	kg/h	161.99	161.99	0.00%	165.77	165.77	0.00%
Reflux flow	kg/h	38,136.40	38,136.40	0.00%	41,927.40	41,927.40	0.00%
Overhead flow	kg/h	2,462.39	2,382.77	−3.34%	452.51	2,332.15	80.60%
Reflux temp.	°C	29.94	29.94	0.00%	30.08	30.08	0.00%
Overhead temp.	°C	57.34	49.80	−15.15%	57.35	64.39	10.93%
Bottom temp.	°C	77.61	71.81	−8.07%	77.79	74.81	−3.98%

3. Modified method and optimisation

We propose modifying this process by adding a tank to store the overhead flow when using a feedstock with a high n-butane content, rather than recirculating the product to the splitter and thus reducing the heat duty. The product produced with the feedstock with a high n-butane concentration adversely affects the i-butane minor product concentration in the minor product storage tank. With the additional tank, however, optimisation is possible because unnecessary energy consumption by the splitter is minimised while the yield and quality of the minor products are maintained. In order to perform this optimisation, we used the optimisation of Model Analysis Tools in Aspen Plus and calculated the minimum reflux rate that can satisfy the required quality and yield of the major and minor products.

3.1 Objective function and constraints

First, we defined the following three constraint functions to identify the objective function and minimised the heat duty using the optimisation function of Model Analysis Tools in Aspen Plus: 1) regardless of the n-butane

content feed, the n-butane composition in the major product should be > 99%; 2) When a feed with a high n-butane content is used, the n-butane content in the overhead flow should also be > 98.5%; 3) When a feed with a low n-butane content is used, the composition of the i-butane overhead flow should be > 75%. The variables to meet the objective function were set at the reflux rate of each splitter. These values are summarised in Table 5.

Table 5. Constraints for the objective function used to minimise the splitter heat duty

Name in PFD	Component	Specification	Condition
HOT-NC4	n-butane	> 99.0%	All cases
OVHD-COM	n-butane	> 98.5%	Beta case
	i-butane	> 75.0%	Alpha case

3.2 Optimisation results and discussion

The optimisation results that satisfy the objective function are listed in Table 6 and Table 7. In the alpha case, the i-butane composition of the overhead flow was 88.448% and the heat duty was reduced by 1116.469 kW. In the beta case, the n-butane content in the overhead flow was 98.683%, while the heat duty was reduced by 7,242.017 kW. We assumed that the process operates for 8,000 h/year and that the operating time of the feeds with alpha and beta case equals 22 and 2 h/day, respectively. The cost of electricity was set to 95 won/kWh, as provided by the utility company, and the exchange rate was assumed to be $1 = 1,100 won. As shown in

Table 8 and 9, the reductions in the energy consumption and operating cost were calculated to be 13.015 GW/year and $1.124 million/year, respectively. These values correspond to reductions of 49.98% and 21.00%, respectively, relative to the current process.

Table 6. Optimisation results for the alpha case

Item	Unit	Name in PFD	Variable name	Initial value	Final value	Variation
Heat duty (Absolute value)	kW	DA-141	Condenser	1719.211	1398.898	-320.313
			Reboiler	2126.860	1658.327	-468.533
		DA-141A	Condenser	1698.736	1573.678	-125.058
			Reboiler	2078.892	1876.328	-202.564
		TOTAL		7623.699	6507.231	-1116.469
Reflux rate	kg/h	DA-141	–	19371.116	15463.318	-3907.798
		DA-141A	–	18781.301	17056.149	-1725.152
Mass fraction	%	HOT-NC4	n-butane	99.631	98.990	-0.641
		OVHD-COM	n-butane	9.286	7.786	-1.500
			i-butane	87.021	88.448	1.427

Table 7. Optimisation results for the beta case

Item	Unit	Name in PFD	Variable name	Initial value	Final value	Variations
Heat duty (Absolute value)	kW	DA-141	Condenser	1953.914	383.834	-1570.081
			Reboiler	2585.387	527.616	-2057.772
		DA-141A	Condenser	1964.226	400.149	-1564.077
			Reboiler	2594.910	544.823	-2050.087
		TOTAL		9098.438	1856.421	-7242.017
Reflux rate	kg/h	DA-141	–	21056.900	3308.149	-17748.751
		DA-141A	–	20870.500	3215.266	-17655.234
Mass fraction	%	HOT-NC4	n-butane	99.586	98.999	-0.587
		OVHD-COM	n-butane	98.183	98.683	0.500
			i-butane	1.153	0.841	-0.313

Table 8. Optimisation results; annual energy consumption reduction and economic gain

Item			Unit	Alpha case	Beta case	Total
Reduction in energy consumption			kW	1116.469	7242.017	8358.485
			GW	8.187	4.828	13.015
Operating time*			h/day	22.000	2.000	24.000
			h/year	7333.333	666.667	8000.000
Economic gain*			$/day	2,121.290	1,250.894	3,372.184
			$ million/year	0.707	0.417	1.124

Table 9. Heat duty and operating cost of the proposed process, compared with those of the current process

Item	Unit	Current process	Proposed process	Reduction rate
Heat duty	kW	16,722.14	8,363.65	49.98%
Operating cost	$/h	669.02	528.52	21.00%

4. Conclusions

We have proposed a means of optimising the iso-/normal gas-splitting process whereby the overhead flow is diverted to a storage tank, rather than being returned to the splitter. This modification would result in reductions in the energy consumption and operating costs of 13.015 GW/year and $1.124 million/year, respectively, corresponding to decreases of 49.98 and 21.00%, relative to the current process. In the modified process, the overhead flow is stored when a feedstock with a high n-butane concentration is used. This can subsequently be sold for additional profit or mixed with a feedstock with a low n-butane concentration feedstock, thus stabilising the n-butane concentration in the feedstock reaching the splitter. In addition, the results of this study can be applied to dynamic simulations based on the modelling of an intelligent process system in a future study.

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