Optimization of Propylene—Propane Distillation Process*

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Dedicated to the 80th birthday of Professor Elemír Kossaczký

Optimization of distillation process, based on the real operating data taken from the factory, was carried out using Aspen Plus simulation engine. A need for the optimization came from the fact that the feed stream quality had been significantly changed recently, together with some of the process parameters. The right combination of pressure and reflux rate was to be found in order to minimize the energy consumption in the reboiler and to obtain the required product purity. The real column efficiency was found and the possibility of column capacity enlargement was tested.

Distillation is an important unit operation in the polypropylene production. The biggest polypropylene producer in Serbia and Montenegro is HIPOL Company from Odžaci, which uses the process based on the Mitsubishi technology [1]. Propylene is polymerized in two mixed flow reactors in homogeneous phase, using a highly active catalyst. High-purity propylene (99.2 mole %) is needed in a reactor section because even small amounts of certain components (such as water, ethane, ethylene, CO, *etc.*) could deactivate the catalyst.

Raw material is the mixture of propylene, propane, methane, ethylene, C-4 fraction, hexane, water, hydrogen, N_2, and some other components from a petrochemical plant. Due to a high feed stream purity propylene has to be separated from propane and the other impurities in the distillation column. After leaving a drying section, the mixture potentially containing small amount of water goes to a distillation column where it is separated to give high-purity propylene.

The aim of this paper was simulation of the propylene—propane distillation column using Aspen Plus 11.1 simulation engine provided by Aspen Technology in order to estimate the influence of the main operating parameters on the product composition and reboiler duty [2, 3]. For this purpose, the process parameters were monitored for 14 h and measured every 30 min. The average value of each parameter (flow rate, composition, *etc.*) was compared with the computer simulation.

THEORETICAL

The Soave—Redlich—Kwong equation of state was the chosen thermodynamic property model, since it can be used for hydrocarbon systems that include common light gases (CO_2, N_2) [2]. The form of the equation of state is

$$P = \frac{RT}{v_\mathrm{m} + c - b} - \frac{a(T)}{(v_\mathrm{m} + c)\,(v_\mathrm{m} + c + b)} \qquad (1)$$

where T is temperature, P pressure, v_m denotes molar volume, and

$$a = \sum_i \sum_j x_i x_j a_{ij} + \sum_i a''_{\mathrm{w}i} x_\mathrm{w}^2 x_i \qquad (2)$$

$$a_{ij} = a_{ji}; a_{ij} = (a_i a_j)^{0.5}(1 - k_{ij}) \qquad (3)$$

$$k_{ij} = a_{ij} + b_{ij}T; k_{ij} = k_{ji} \qquad (4)$$

$$b = \sum_i x_i b_i \qquad (5)$$

$$c = \sum_i x_i c_i \qquad (6)$$

In these equations x_i and x_j are mole fractions of component i and j in the mixture. SRK model has several important corrections comparing to the Redlich—Kwong—Soave model, which is based on the same equation. First of all, a volume translation concept

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introduced by *Peneloux et al.* [4] is used to improve molar liquid volume calculated from the cubic equation of state. Further, the phase equilibrium calculations for mixtures containing water are improved by using the Kabadi—Danner modification for the mixing rules [5]. The term $\sum_i a''_{wi} x_w^2 x_i$ is used only when the Kabadi—Danner option is enabled, where

$$a_{ij} = a'_{wj}; \quad a'_{wj} = (a_w a_j)^{0.5}(1 - k_{wj}) \tag{7}$$

$$a''_{wi} = G_i \left[1 - \left(\frac{T}{T_{cw}}\right)^{0.8}\right] \tag{8}$$

In these equations w represents water and j hydrocarbon; k_{wj} is obtained from experimental data; T_{cw} is the critical temperature of water; G_i is the sum of the group contribution of different groups which make up a molecule of hydrocarbon. For pure components parameters a_i, b_i, and c_i are given by the following equations

$$a_i = f(T, T_{ci}, P_{ci}, \omega_i) \tag{9}$$

$$b_i = f(T, T_{ci}, P_{ci}) \tag{10}$$

$$c_i = 0.40768 \left(\frac{RT_{ci}}{P_{ci}}\right)(0.29441 - z_{RAi}) \tag{11}$$

T_{ci}, P_{ci} being the critical temperature and pressure, and ω_i, z_{RAi} correspond to acentric and compressibility factor of the pure component i, respectively.

EXPERIMENTAL

The propylene—propane distillation column is schematically shown in Fig. 1. Because of the high product purity and the low relative volatility, the number of stages required for this separation is very high. Two towers are installed because a single tower would be too tall (C-001 and C-002), C-001 having 122 stages (including reboiler) and C-002 with 121 stages (including condenser). Two pumps are noted as P-001 and P-002. The reboiler, condenser, and reflux vessel are noted as E-003, E-004, V-003, respectively. The feed stream is inserted in the column C-001 on the stage 85,

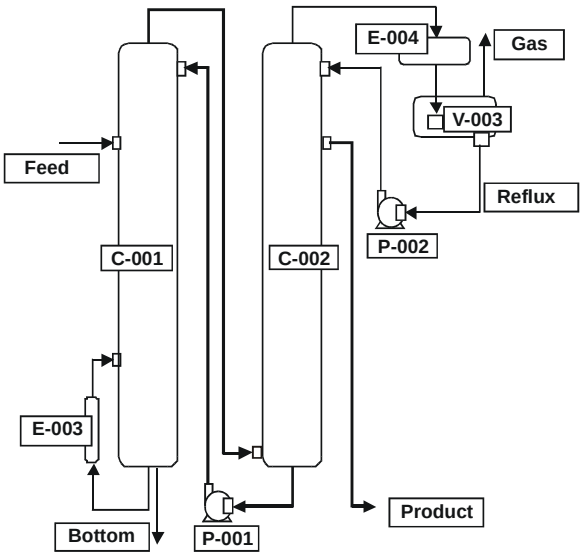

Fig. 1. Schematic picture of the propylene—propane distillation column.

which corresponds to the stage 156 in the one-column simulation model (numbered from the top, starting with the top stage) and the product stream leaves C-002 column at the stage 12 (also numbered from the top, but starting with the condenser). A reason for this nonconventional withdrawal of the distillate stream is the fact that there is a high concentration of some light components at the top of the column, which could later on poison the catalyst. The column internals data [1] as well as the temperature and pressure ranges measured in the column are given in Table 1. The feed stream is at 2.3 MPa and 17 ℃ and it is 100 % liquid.

Table 2 shows the process parameters necessary for the computer simulation. As mentioned before, these values are average for the period of 14 h of the column operation. The flow rates, pressure and temperature values were measured in-line and taken directly from the control board of the distillation process, while the sample composition of each material stream was analyzed using a GC-FID in the laboratory.

A computer simulation was applied for the descrip-

Table 1. Column Internals Data and Temperature and Pressure Ranges Measured in the Column

Diameter/m	2.1	
Number of stages	241	
Tray type	Sieve + valve (each fourth plate is with valves), 2 passes, hole diameter 0.039 m, 388 holes per tray	
Tray spacing/m	0.45	
Weir height/m	0.0545	
Downcomers	Side	Centre
Width at a top/m	0.35	0.28
Width at a bottom/m	0.35	0.28
Clearance/m	0.0445	0.0445
P/MPa	1.595—1.756	
t/℃	35.7—49.2	

Table 2. Measured and Simulated Material Stream Composition

Stream component	F/(kg h^{-1})		D/(kg h^{-1})		B/(kg h^{-1})		G/(kg h^{-1})	
	Measured	Simulated	Measured	Simulated	Measured	Simulated	Measured	Simulated
Hydrogen	0.13	0.13	–	–	–	–	0.13	0.13
Nitrogen	1.76	1.76	–	0.01	–	–	1.76	1.75
Ethane	0.16	0.16	–	0.09	–	–	0.16	0.07
Propane	178.73	178.73	37.57	37.87	141.10	140.81	0.06	0.05
Propylene	5304.48	5304.48	5262.43	5262.03	28.16	28.45	13.89	14.01
Butane	2.20	2.20	–	–	2.20	2.20	–	–
Heptane	8.54	8.54	–	–	8.54	8.54	–	–
Total	5496	5496	5300	5300	180	180	16	16

tion of the distillation column. RADFRAC unit operation model from the Aspen Plus model library was used [2, 3, 6]. RADFRAC is a rigorous model for simulating all types of multistage vapour-liquid fractionation operations. Although RADFRAC assumes equilibrium stages, it is possible to specify Murphree efficiency to match plant performance. Two columns used in the polypropylene plant are considered as one by the simulation program since the column 2 acts as an extension of the column 1 (the column division into two parts comes as a physical restriction of the RADFRAC unit operation model).

The column efficiency was unknown parameter. For this system propylene was considered as a light key component and propane as a heavy key component. In Design Specs of the Flowsheeting Options menu propylene and propane mass fractions in the distillate and bottom stream were used as design specifications while the column efficiency was the manipulating variable. Determined stage efficiency was used for all other simulation runs.

The reflux rate was the manipulating variable in a sensitivity analysis performed in order to estimate its influence on some important process parameters such as the reboiler duty and the product purity. These simulations were performed with the aim to investigate the influence of feed flow rate increase on the propylene production.

A tray rating calculation was performed in order to estimate how the feed flow rate variation will affect the column hydrodynamics parameters such as the flooding factor.

RESULTS AND DISCUSSION

The column efficiency was varied from 30 % to 100 %. A target value for the propylene (propane) mass fraction in the distillate stream was 0.9929 (0.00709) and in the bottom stream 0.1564 (0.7839). As a result, the efficiency was found to be 40.75 %, relatively low but realistic value, according to [7]. Fig. 2 shows the variation of propylene mole fraction in the distillate ($x_{\mathrm{D,propylene}}$) with the column efficiency (η).

With the overall efficiency determined simulation

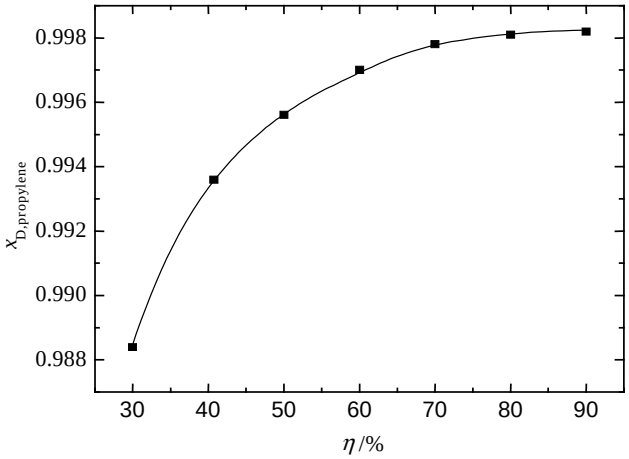

Fig. 2. The propylene mole fraction in the distillate as a function of the column efficiency.

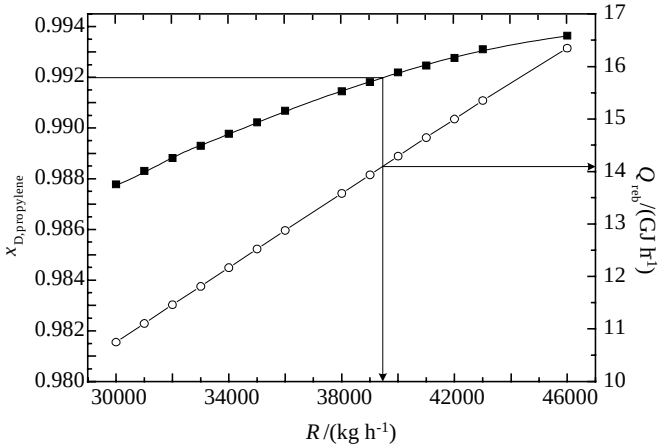

Fig. 3. Influence of the reflux flow rate on the reboiler duty (○) and product purity (■).

was run in order to obtain the material streams compositions. Results of this simulation are also given in Table 2 for comparison with the real process data. It is worth mentioning that the simulation results fit very well the measured data.

During sensitivity analysis, based on variation of

Table 3. Column Process Parameters Variation with the Feed Flow Rate

F/(kg h^{-1})	R/(kg h^{-1})	Q_{reb}/(GJ h^{-1})	(Q_{reb}/F)/(GJ kg^{-1})
5496	43211	15.43	2.81
7000	56200	19.98	2.85
9000	72000	25.73	2.86

the reboiler duty (Q_{reb}) and the propylene purity ($x_{\mathrm{D,propylene}}$) with the reflux flow rate, the independent variable R was varied from 30000 kg h^{-1} to 46000 kg h^{-1}. Fig. 3 summarizes the results of this simulation. As expected, variation of the reboiler duty with the reflux flow rate was linear. It is obvious that the energy consumption in the reboiler is reduced decreasing the reflux flow rate. On the other hand, this decrease affects the product purity by reducing it. As it is shown in Fig. 3, the minimum reflux flow rate to obtain the required distillate purity of 99.2 mole % of propylene is 39600 kg h^{-1} ($\eta = 0.4075$), to which corresponds the reboiler energy consumption of 14.15 GJ h^{-1}.

In order to investigate the column capacity the distillate to feed and bottom to feed mass flow ratios were kept unchanged ($D/F = 0.96$, $B/F = 0.033$) while the reflux flow rate was adjusted to give 99.3 mass % of propylene in the distillate. The reflux flow rate, reboiler duty, and specific heat consumption (heat consumption per ton of feed, Q_{reb}/F) are presented in Table 3 for the feed flow rates of 5496 kg h^{-1}, 7000 kg h^{-1}, and 9000 kg h^{-1}. The simulation results show that the specific heat consumption is about the same for all the feed stream flow rates. Working on long terms this could be quite profitable. But before drawing a general conclusion, real column flexibility should be checked. It means that the tray rating calculation (with detailed constructive description of a plate) should be done in order to obtain a value of the flooding factor which should not exceed unity.

The tray rating calculation gives the flooding factor (defined as a ratio between the actual vapour velocity and the vapour velocity, at which the flooding point is reached, FF) for a tray in the column as well as the maximum flooding factor for the entire column. This calculation was tested for the selected feed stream flow rates of 5496 kg h^{-1}, 7000 kg h^{-1}, and 9000 kg h^{-1}. The most important input hydraulic parameters of a plate column used during the calculation are given in Table 1. Fig. 4 shows the flooding factor as a function of the plate number (N_{S}). The maximum flooding factors for the three selected flow rates were 0.6071, 0.7872, and 1.014, respectively. Theoretically, the column could be operated even at a feed flow rate a bit lower than 9000 kg h^{-1}. But reaching this point, another restriction should be taken into account: the reboiler and condenser heat transfer area as well as the heating and cooling fluid flow rates and temperatures.

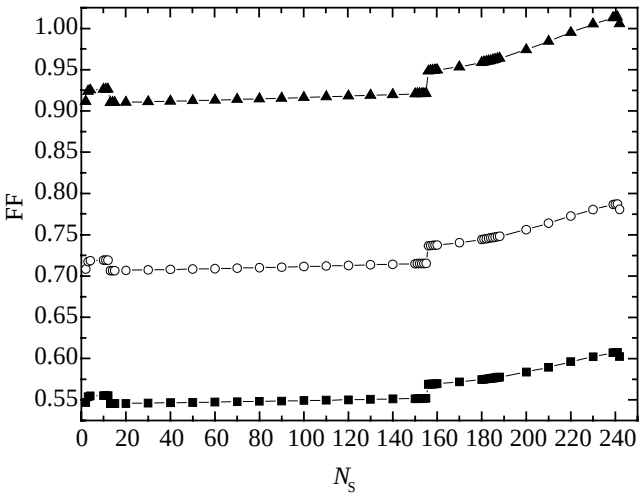

Fig. 4. The flooding factor as a function of the plate number for the feed flow rates of 5496 (■), 7000 (○), and 9000 (▲) kg h^{-1}.

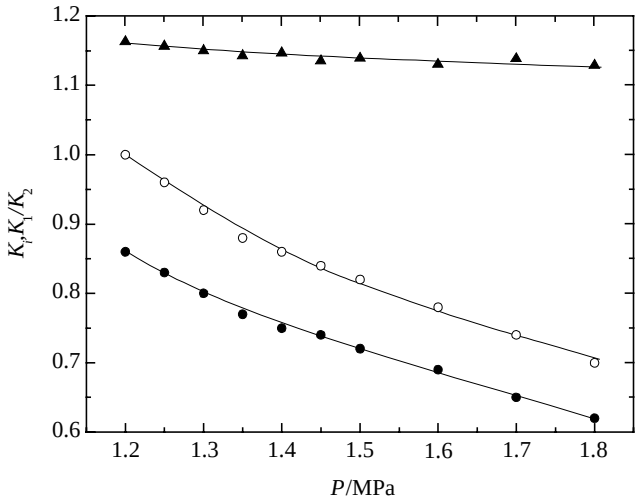

Fig. 5. Pressure influence on the propylene—propane phase equilibrium at $t = 25$ ℃. ● K_2 (factor for propane), ○ K_1 (factor for propylene), ▲ K_1/K_2.

A sudden flooding factor decrease between the stage 12 and 13 is a consequence of the distillate stream withdrawal from the stage 12, which significantly reduces the liquid flow rate in the column. A similar situation occurs between the stage 156 and 157: the flooding factor increases due to the feed stream input on the stage 156.

Another possibility for the operation costs reduction is a pressure reduction in the column. Apart from the boiling point temperature decrease, the pressure reduction influences the quantity of propylene in the vapour phase for propylene—propane mixtures by increasing it. This behaviour is shown in Fig. 5, for the temperature of 25 ℃ [8]. The propylene—propane relative volatility (a ratio between the propylene and

Table 4. Pressure Influence on the Energy Consumption of the Distillation Process

P/MPa	t_{top}/℃	t_{bottom}/℃	R/(kg h^{-1})	Q_{reb}/(GJ h^{-1})
1.595	36.7	50.5	43211	15.43
1.4	31.4	45.4	39200	14.31
1.2	25.3	39.3	35650	13.29

propane K factors) increases with the pressure decrease.

The following analysis should give a path for the pressure adjustment at the top of the column. If the goal is to obtain the distillate with 99.3 mass % of propylene, then the adjusted reflux flow rates for obtaining this purity are given in Table 4 (for the pressures at the top of the column of 1.4 MPa and 1.2 MPa and D/F and B/F unchanged). Also, Table 4 shows the temperatures at the top and the bottom of the column, together with the reboiler heat duty. However, some process limitations, such as the lowest cooling water temperature which can be achieved, do not permit to operate under the pressure at the top of the column lower than 1.2 MPa. On the other hand, working under the pressure of 1.4 MPa would result in significant energy saving (14.31 GJ h^{-1} instead of 15.43 GJ h^{-1}).

SYMBOLS

a	parameter of SRK equation of state	J mol^{-1}
B	bottom mass flow rate	kg h^{-1}
b	parameter of SRK equation of state	m^3 mol^{-1}
c	parameter of SRK equation of state	m^3 mol^{-1}
D	distillate mass flow rate	kg h^{-1}
F	feed mass flow rate	kg h^{-1}
FF	flooding factor	
G	the sum of the group contribution of groups which make up a molecule of hydrocarbon	
G	gas mass flow rate	kg h^{-1}
g	mass fraction	
K	K factor ($K = y/x$)	
k	binary interaction coefficient for SRK equation of state	
N_S	tray number	
T	thermodynamic temperature	K
t	Celsius temperature	℃
P	pressure	MPa
Q	heat duty	GJ h^{-1}
R	gas constant in eqns (*1*) and (*11*)	J K^{-1} mol^{-1}
R	reflux mass flow rate	kg h^{-1}
v_m	molar volume	m^3 mol^{-1}
x	mole fraction in liquid phase	
y	mole fraction in vapour phase	
z_{RA}	Rackett's compressibility factor	

Greek Letters

η	Murphree efficiency
ω	acentric factor

Subscripts

bottom	bottom of the column
c	critical
m	molar
i, j	components
reb	reboiler
top	top of the column
w	water

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