SIMULATION AND DESIGN OF AN ENERGY EFFICIENT 1,3-BUTADIENE RECOVERY UNIT

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An extractive distillation unit has been designed and simulated focusing on the energy efficient recovery of 1,3-butadiene from a crude C4 fraction applying the N-methylpyrrolidone solvent extraction technology. For the the binary interactions between every component in feed and solvent a mix of literature values and values estimated by Aspen were used. The steady state simulation was optimized by a manual sensitivity analysis and good agreement was obtained with plant data with an 80 kton/year 1,3-butadiene production capacity. Pinch analysis is applied to maximize the process-to-process heat recovery and to minimize the utility (energy) requirements, reducing the external energy requirement with over 35%. Our simulations further show that employing a divided wall column instead of the classically used distillation columns for the separation of propyne and 1,2-butadiene from 1,3-butadiene does not lead to an improvement in energy efficiency.

1. INTRODUCTION

1,3-Butadiene is a valuable intermediate in the fabrication of polymers and rubbers. It is produced commercially by three processes: steam cracking of naphtha, catalytic dehydrogenation of n-butane or n-butene, and oxidative dehydrogenation of n-butene. Currently the steam cracking process accounts for 95% of the world's butadiene supply. Next to ethylene and propylene, a naphtha steam cracker also produces a C4 cut, typically containing about 40 wt% of butadiene, that can be purified in a 1,3-butadiene recovery unit. In Table 1 a typical composition of the crude butadiene feed is given. Separation of 1,3-butadiene from the C4-cut by conventional distillation is not possible due to the formation of several azeotropes and very close boiling points of most of the components, as can be seen from Table 1. The alternative process for separation of 1,3-butadiene from the C4-cut is extractive distillation or liquid-liquid extraction. The liquid-liquid extraction technology has problems when higher concentrations of α-acetylenes (ca. 100 ppm of vinyl acetylenes) as a result of foam formation, and therefore cannot be used for the present case.(Ullmann, 2010) Several commercial processes are available that employ extractive distillation. Extractive distillation is defined as distillation in the presence of a miscible, high boiling, relatively nonvolatile compound (i.e., the solvent) which forms no azeotrope with other components in the mixture. This separation technique is widely used in chemical and petrochemical industries for separating azeotropic, close-boiling and low relative volatility components from the mixture. In extractive distillation, the solvent is chosen to interact differently with the components of the original mixture, thereby, altering their relative volatilities. Since these interactions occur predominantly in the liquid phase, the solvent is continuously added close to the top of the extractive distillation column such that an appreciable amount of solvent is present in the liquid phase on all the trays below. In literature several promising solvents are presented which allow to separate butadiene from the C4 cut. These solvents are N-methylpyrrolidone [NMP] (Klein and Weitz, 1968, Hausdorf.B et al., 1968), dimethylformamide [DMF] (Takao, 1966, Takao, 1979), acetonitrile [ACN] (Lei et al., 2002), furfural (Stryjek and Luszczyk, 1978), dimethylacetamide [DMAC] (Ullmann, 2010). Table 1 compares the relative volatilities of these different components at 50°C to 1,3-butadiene in the different solvents. The relative volatility α is defined as the ratio of the vapour-liquid equilibrium constant for two components:

$$\alpha = \frac{y_i/x_i}{y/x} = \frac{K_i}{K} \tag{1}$$

with α the relative volatility of the specified component i to 1,3-butadiene, y_i the vapor-liquid equilibrium concentration of component i in the vapor phase, x_i the vapor-liquid equilibrium concentration of component i in the liquid phase, y the vapor-liquid equilibrium concentration of 1,3-butadiene in the vapor phase, and x the vapor-liquid equilibrium concentration of 1,3-butadiene in the liquid phase. According to the results presented in Table 1 NMP is the best solvent. NMP has some additional advantageous over the others, e.g. the low solvent losses, very low fouling tendency and high purity of the obtained 1,3-butadiene. Therefore the design of the 80 kton/year 1,3-butadiene recovery unit is based on the NMP technology developed by BASF(Kindler and Puhl, 2002, Bohner et al., 2006). The focus of this project is on the development of an energy efficient purification section for the crude C4 stream. Two designs of this recovery unit will be compared, i.e. a design with a conventional distillation section (Kindler and Puhl, 2002) and a design that employs the recently patented divided wall technology (Bohner et al., 2006). Special attention is paid to the selection of reasonable binary interaction coefficients between feed and solvent, because the latter strongly affect the output of the simulation. The pinch method is used to maximize the internal heat integration in the recovery unit.

Table 1: C4 fraction: composition, individual boiling points, and relative volatilities at 50°C compared to 1,3-butadiene (Ullmann, 2010)

Component	Wt %	Boiling point °C	α_{NMP}	α_{DMF}	α_{ACN}	α_{DMAC}	$\alpha_{furfural}$
Propane	0.05	-42.1	n.a.	n.a.	n.a.	n.a.	n.a.
Propadiene	0.01	-33.2	n.a.	n.a.	n.a.	n.a.	n.a.
Propyne	0.07	-4.6	0.8	0.7	0.7	0.7	0.7
1,2-butadiene	0.70	10.9	0.7	0.7	0.7	0.7	0.7
1,3-butadiene	40.50	-0.2	1.0	1.0	1.0	1.0	1.0
n-butane	6.50	-11.2	3.7	3.4	3.1	3.1	2.9
i-butane	3.00	-6.4	3.7	3.4	3.1	3.1	2.9
1-butene	12.30	1.1	2.4	2.2	1.9	2.1	1.8
2-butene	8.20	-6.5	1.9	1.8	1.6	1.7	1.2
Isobutylene	28.00	9.9	1.6	1.6	1.5	1.5	1.3
t-butyne	0.20	-23.2	0.4	0.4	0.5	0.4	0.5
Vinyl-Acetylene	0.50	3.0	0.2	0.2	0.4	0.2	0.4
C5-fraction	0.03	> 11	n.a.	n.a.	n.a.	n.a.	n.a.

2. PROCESS DESCRIPTION

The block flow diagram of butadiene extraction process is shown in Figure 1. This process include two major process steps: first an extractive distillation section followed by a conventional distillation section. The extractive distillation section consists of a first extractive distillation column, the so-alled main washer, a second extractive distillation column, the after washer, and a degassing column. Butanes and butenes, which have the smallest solubility in NMP, are separated as the overhead product (raffinate) of the extractive distillation section. The vapor stream consisting mainly of 1,3-butadiene and C4-acetylenes is sent to the second extractive distillation step. In this tower the acetylenic components are removed by means of fresh NMP. Crude butadiene is withdrawn as the overhead product of the second extractive distillation step. The C4-acetylenes are fully

absorbed by NMP and are withdrawn from the degassing section. In the degassing section dissolved hydrocarbons are completely removed from the solvent.

Crude butadiene obtained from the extractive distillation is further purified in two subsequent distillation towers. The conventional distillation section consists of the propyne distillation column and the butadiene distillation column. In the first distillation tower propyne together with some 1,3-butadiene for dilution is withdrawn as the overhead product. In the second distillation tower a mixture containing 1,2-butadiene and C5-hydrocarbons are separated as the bottom product. The 1,3-butadiene product is withdrawn from the overhead of the final distillation tower.
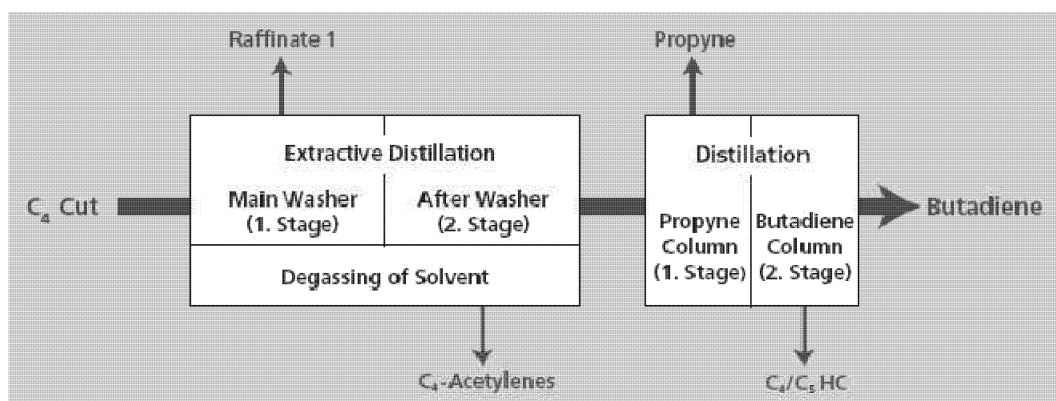

Figure 1: Block diagram of the NMP process

Figure 2 shows the simplified process flow diagram of the 1,3-butadiene extraction process. The separation process is divided in three parts: the extractive distillation section, the degassing section and the conventional distillation section. The extractive distillation zone operates at a pressure of about 4 bar. The C4 feed is available at 25°C and should be heated up to 60°C before injection in the main washer. The vaporized C4-cut enters the main washer at the bottom together with the top gas from the rectifier and is counter-currently washed with NMP. 1,3-Butadiene is almost completely absorbed in this tower. The overhead product from the main washer contains most of the propane, propene, propadiene, butanes and butanes present in the C4-cut. In the upper part of the rectifier, the more volatile butene is stripped from the solvent by a counter-current vapor stream of the more soluble butadiene rising from the bottom. The gaseous mixture of 1,3-butadiene and butene leaves the rectifier top and is send back to the bottom of the main washer. The concentration of 1,3-butadiene in the vapor rises to its maximum between the rectifiers upper and lower part. A butadiene-rich side-stream is withdrawn from the rectifier and fed to the bottom of the after-washer. The solvent (NMP) with approximately 8.3 wt% water, is fed to the top of the main washer. The solvent withdrawn from the bottom of the main washer is pumped to the top of the rectifier. In the after washer vinylacetylene and ethylacetylene are removed from 1,3-butadiene. These C4-acetylenes are more soluble in NMP than 1,3-butadiene and are removed counter-currently with fresh solvent that is fed to the top of the column. The C4- acetylenes absorbed in the solvent are drawn from the bottom of the after-washer and transferred by the after-washer pump to the rectifier. Water which is presented in the overhead vapor of this tower is separated from the organic phase in the bootleg of an accumulator. Note that the three columns (main washer, rectifier and after washer) are strongly intertwined, resulting in very large recycle streams in between them.

In Figure 2 a single divided wall column is used in the conventional distillation section to purify the 1,3-butadiene. If 2 columns are used for purifying the 1,3-butadiene then first propyne is separated from the butadiene. The removal of propyne is necessary because of its explosive character and that it can cause serious problems in 1,3-butadiene polymerization processes. In the following tower 1,2-butadiene and heavier

components are then separated from the 1,3-butadiene stream. The conventional distillation section operates at a pressure of about 7 bars. The purified 1,3-butadiene is retrieved in stream T4.

In the conventional distillation section there is no use for an extraction solvent. The solvent is hence separated from the other components and sent to the degassing section for solvent recovery. Since stream B5 contains pure solvent, i.e. NMP and water, it can of course be recycled to the main washer and the after washer. In order not to overload the flow diagram, this recycle stream is not indicated in the flow diagram. Moreover, the solvent recovery is approximately 100%, so virtually no make-up solvent is necessary. Note that the degassing section is also used to remove the small amount of hazardous ethyl- and vinyl acetylene. Other C4 components that are dragged along in stream B2 are send back to the extractive distillation section via stream R3. This gaseous recycle stream, which receives extra energy from a compressor, provides the reboiler heat needed for the extractive distillation. Hence, no extra reboiler is required in the extractive distillation zone. The degassing section operates at a pressure of about 1.5 bar. The compressor that increases the pressure of stream R3 from 1,5 to 4 bar is a two-stage compressor with intercooler.

Figure 2: Simplified process flow diagram of 1,3-butadiene extraction process with divided wall column

3. MODELING

3.1 Feedstock and product specifications

In an industrial naphtha steam cracker the composition of the crude C4 fraction will vary depending on the feedstock, the process conditions and the separation train, e.g. front-end hydrogenation (Ullmann, 2010). In the present study the composition of the crude C4 cut is assumed fixed during the 8000 hrs operating time. The composition of the crude C4 cut has been given in Table 1. Our objective is to produce polymer grade 1,3 butadiene with a purity of 99.5 wt%. The product specifications of the 1,3-butadiene are listed in Table 2. The following utilities are assumed to be available on the production site: low pressure steam of 4.5 bar, medium

pressure steam of 17 bar and the cooling water has a temperature of 24°C. A temperature approach, i.e. temperature difference between the outlet and the inlet streams, of 10°C is assumed. The desired recovery of 1,3-butadiene is set to 98 wt%.

Table 2: Overall recovery unit product specifications for the polymer grade 1,3-butadiene stream

Component	Specification (weight based)
1,3-buatdiene	min. 99,5 wt%
1,2-butadiene	max. 25 ppm
Propadiene	max. 20 ppm
Methyl-acetylene	max. 20 ppm
Vinyl-acetylene	max. 20 ppm
Total acetylenes	max. 20 ppm
C5-hydrocarbons	max. 1000 ppm

3.2 Simulation methodology

The numerous recycle stream makes that the simulation needs to be build-up step by step. First of all the 1,3-butadiene extraction unit is divided into two separate parts: the extractive distillation section containing the extractive distillation columns that use NMP as solvent and the conventional distillation section (without NMP solvent). This detachment was made because in both sections a different equation of state needs to be used to describe the interactions between the different components.

To avoid convergence problems as much as possible, each simulation project was divided into different steps. First, the different columns were simulated and optimized as separate units, starting with the main washer, followed by the rectifier, after washer, degasser and solvent washer. Subsequently, the different columns were connected: first the main washer was connected to the rectifier, subsequently the after washer was added, etc. To improve the separation in the different columns and to obtain the required specifications, numerous sensitivity analyses were carried out. These analyses often suffered from severe convergence problems. The convergence stability was poor, mainly caused by the many recycle streams that were integrated in the process (e.g. rectifier). Therefore, sensitivity analyses were often conducted manually, changing the process parameters in very small steps. Column temperatures required constant monitoring during the simulation because stages dried up when recycle streams were not fed at appropriate stages. Note that the NMP recycle could not be closed in our simulations because of convergence issues, and hence, the NMP recycle has been closed artificially.

3.3 Property method and Calculation of Interaction coefficients

The selection of a proper thermodynamic property method, i.e. a proper equation of state with attention to the components and process conditions, is crucial for each simulation. For the extractive distillation the Non-Random Two-Liquid (NRTL) property method is used in agreement with previous work (Saffari et al., 2005). Binary parameters that are not available in the NRTL database are estimated by use of the UNIFAC model. The Peng-Robinson equation of state is selected for the conventional separation section where propyne and 1,2-butadiene need to be separated from 1,3-butadiene. Next to the values calculated by Aspen also literature values for the interaction coefficients were considered (Saffari et al., 2005). The only relevant data found in literature (Ullmann, 2010) for validation of the interaction coefficients are the volatilities relative to 1,3-butadiene of the main components in the C4-cut. Table 3 shows that significant differences exist between the values found in literature and these obtained from Aspen or using the interaction coefficients of Saffari et al. The relative volatilities of butane, 1-butene, isobutylene, 2-butene are all higher than 1, and hence it can be expected that butanes and butenes will be separated from 1,3-butadiene at the top of the first extractive distillation. Working with the interaction coefficients of Saffari et al. does not seem advisable because at 20°C the relative volatilities

of isobutylene and 2-butene are smaller than 1, and hence, these components will not be removed from 1,3-butadiene in the main washer. Safari et al. adapted the interaction parameters in such way that the more volatile and the less volatile components are separated easier from 1,3-butadiene than what is observed experimentally. The only component for which a better agreement is observed with the literature values than those calculated with Aspen is propyne. The relative volatilities of propyne are closer to 1 for the NRTL-parameters by Saffari et al., what is in agreement with experimental data. Although overall the NRTL-parameters from Aspen give a better agreement with the literature values these are far from perfect. For 1,2-butadiene and propadiene interaction parameters are not available in the Aspen database and cannot be estimated. As a result the 1,2-butadiene values are not corresponding with the literature data. If as solvent NMP is chosen methylacetylene will be separated from 1,3-butadiene together with butanes and butenes instead of going to the conventional distillation columns with 1,3-butadiene. Therefore we have adjusted the NRTL parameters in Aspen for some of the components based on our findings. The observation that excellent agreement is observed between the relative volatilities calculated with Aspen and those found experimentally when DMF instead of NMP is used as solvent helped significantly for adjusting the NRTL-parameters for NMP in Aspen. The calculated relative volatilities with these modified NRTL-parameters agree well with the experimentally observed values, as can be seen from Table 3.

Table 3: relative volatilities compared to 1,3-butadiene (Ullmann, 2010)

	$\alpha_{NMP, 20°C}$				$\alpha_{NMP, 50°C}$			
	Aspen	Safari et al.	Aspen modified	Exp.	Aspen	Safari et al.	Aspen modified	Exp.
Propyne	-	-	-	-	1.5	1.1	0.9	0.8
1,2-butadiene	-	-	-	-	0.3	0.4	0.7	0.7
1,3-butadiene	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
n-butane	2.1	8.7	3.5	3.8	2.3	11.2	3.5	3.7
i-butane	2.1	8.7	3.5	3.8	2.3	11.2	3.5	3.7
1-butene	1.6	1.5	2.1	2.4	1.7	1.6	2.1	2.4
2-butene	1.4	0.8	1.8	2.0	1.5	1.5	1.7	1.9
Isobutylene	2.0	0.9	2.2	2.5	-	-	-	-
t-butyne	-	-	-	-	0.7	0.6	0.5	0.4
Vinyl-Acetylene	-	-	-	-	0.5	0.3	0.7	0.8

4. RESULTS AND DISCUSSION

4.1 Steady state simulation of extractive distillation section

The extractive distillation section has been simulated according to the procedure discussed in section 3.1 with the interaction coefficients determined by Aspen, with those from Saffari et al. and using modified Aspen interaction coefficients. Using the values from Saffari et al. it was not possible to reach the desired recovery and purity. A recovery of 85,27% and a purity of 75,60 % are the best results which can be obtained with the fully optimized process conditions. This is caused by the huge amounts of isobutylene and 2-butene remaining in the top product of the after washer, which is expected based on the relative volatilities reported in Table 3. If the NRTL-parameters from Aspen are used 1,2-butadiene was removed with the vinyl-acetylene stream (T5) instead of in the top-stream (T2) of the second extraction column. Propadiene on his behalf could not be distilled from the 1,3-butadiene cut in the first extraction column. Therefore in all further simulations the modified Aspen NTRL-parameters were used.

In order to obtain an overall 1,3-butadiene recovery of more than 98%, the amount of 1,3-butadiene in the top stream of the main washer must be limited to 1% of the total amount present in the feed. Further losses of 1,3-

butadiene occur in the washing column and the purification section. For both the main and after washer NMP are fed at the top of the column. The pressure in the main washer and the after washer was determined in such a way that cooling water could be used in for condensing the overhead streams of these two columns. Table 4 summarizes all the results for the extractive distillation section. What is remarkable is that both the purity and the recovery of the distilled 1,3-butadiene can both be improved by decreasing the solvent flow to the after washer column. This unexpected result is only hampered when the flow becomes so low that the upper trays of the column dry up. This effect will occur faster when using a lower hydrocarbon feed to the column. The reboiler and condenser duties of the extractive distillation section agree well with the values from an industrial unit.

Next to duties for reboiler and condenser also energy is required to operate equipment shown in Figure 2 such as pumps, a 2 stage compressor and heat exchangers. The duties for other equipment per ton 1,3-butadiene are respectively: 2.9 GJ for heating stream B2, 3.2 GJ for heating stream R2, 0.6 GJ for the 2 stage compressor.

Table 4: Configuration of the extractive distillation section and degassing zone

	Main washer	Rectifier	After washer	Degasser	Solvent washer
Number of trays	50	28	35	10	5
Feed tray	45	1	35	1	5
Solvent feed tray	4	-	4	-	1
Pressure [bar]	4	4	4	4	5
Condenser duty [GJ/ton butadiene]	2.22	-	3.86	-	0.23
Reboiler duty [GJ/ton butadiene]	-	-	-	4.47	-
Solvent to feed ratio [kg/kg]	9.0	-	0.2	-	-
Temperature top [°C]	36	57	37	99	25
Temperature bottom [°C]	57	85	53	145	131

The top stream of the after washer T2 contains next to 1,3-butadiene, of 0.2 wt% propyne, 2.3 wt% 2-butene and 1.6 wt% 1,2-butadiene. This stream is sent to the conventional distillation section.

4.2 Divided wall versus conventional distillation

In the second part of this simulation the 1,3-butadiene rich product stream coming from the extractive distillation section is further purified to obtain the product specifications set in Table 2. The feasibility of using the relatively new divided wall column (DWC) technology for the 1,3-butadiene recovery unit was explored for the separation of the tertiary mixture eluting from the extractive distillation section. Recent patents claim that the two columns in the conventional distillation zone of the NMP process can be replaced by a single divided wall column. (Bohner et al., 2006) The main reasons to consider these types of columns are its potential to save energy (due to the elimination of one reboiler and condenser) and reduce investment costs (due to the elimination of one column). The latter is however only true for certain feed conditions and relative volatilities of the products. (Agrawal and Fidkowski, 1998) This deficiency originates from the second law of thermodynamics. A fully thermally coupled configuration receives all heat at the highest temperature and rejects it at the lowest temperature. This often results in a lower thermodynamic efficiency compared to the direct or indirect sequences of distillation columns. (Agrawal and Fidkowski, 1998)

As stated previously the Peng-Robinson equation of state is used to design the propyne and butadiene column. Short-cut methods provide first estimates for the optimal reflux and the number of theoretical plates. Aspen Plus is then used to determine the number of stages, the reflux and the number of the feed stage based on the desired recoveries of the key-components. The results for the optimized propyne and butadiene column are given in

Table 5 and the reboiler duties agree well with what is found in industrial butadiene recovery section. All specifications for the 1,3-butadiene product are met and the recovery of 1,3-butadiene is 99%.

Table 5: Configuration of the conventional distillation section

	Propyne column	Butadiene column
Number of trays	55	75
Product tray	22	42
Pressure [bar]	6	5
Condensor duty [GJ/ton butadiene]	0.57	3.31
Reboiler duty [GJ/ton butadiene]	0.61	3.29
Temperature top [°C]	36.4	45.1
Temperature bottom [°C]	52.6	55.2

The DWC can be considered as the thermodynamically equivalent of a Petlyuk column (Petlyuk et al., 1965) and was simulated as such in Aspen. The simulation results were compared with results obtained with the classical configuration that used two conventional distillation columns, i.e. the propyne and butadiene column. According to the literature (Bohner et al., 2006) the energy consumption of a DWC is 10% less than the energy consumption of the conventional distillation section and the DWC consist of 40 up to 70 theoretical plates. The simulation was carried out with 70 stages as it was found that a lower number of trays made it hard to reach the column specifications. The stages in the divided wall section, which is modeled as a prefractionator, are numbered according to their corresponding location in the main column.

Simulation showed that with 10% reduction of the heat input the obtained 1,3-butadiene purity and recovery do not meet the desired specifications, i.e. a purity of 99.3% and a recovery of 98.5% were obtained respectively. As can be seen in Figure 3 the optimal feed stage for the DWC is located on plate 27, while the wall is located between stage 12 and 55. The only solution to reach the desired purity of 1,3-butadiene is to increase the reboiler duty to at least 9 GJ per ton 1,3-butadiene.
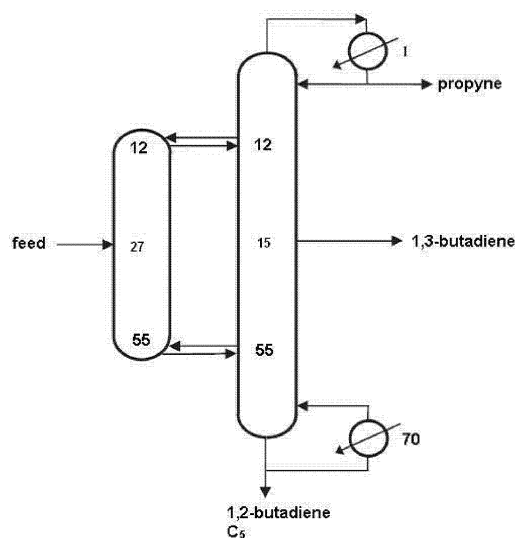

Figure 3: Divided wall column modelled as a Petlyuk column for purification of
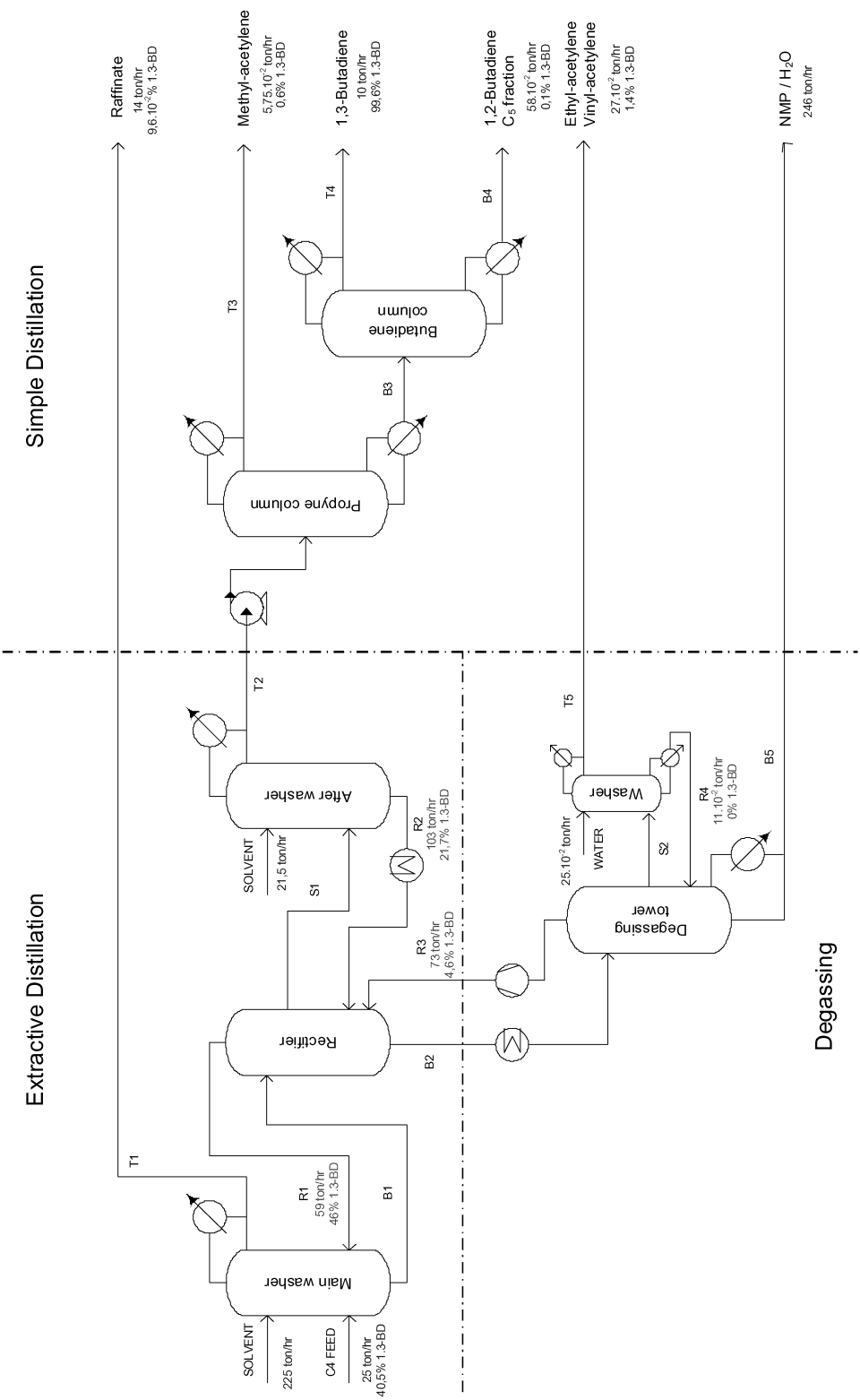
Figure 4: Calculated mass flows for the optimized 1,3-butadiene recovery unit with a conventional distillation section

4.3 Optimization and pinch analysis

Figure 4 shows the calculated mass flows for the optimized 1,3-butadiene recovery unit with a conventional distillation section. This optimization is the results from the separate optimization of the extractive distillation/degassing section and the conventional distillation section. The overall recovery for 1,3-butadiene is 98.7%, while the purity of the 1,3-butadiene stream is 99.6 wt%.

The methods available for energy targeting of heat exchanger networks can be divided in mixed integer linear or non-linear formulations (Jezowski et al., 2000, Asante and Zhu, 1997, Yee and Grossmann, 1990), or are based on the pinch method (Linnhoff and Hindmarsh, 1983, Linnhoff, 1993, Douglas, 1988, Seider et al., 1999, Smith, 2005). The former are capable of providing the global optimal solution to these problems and may ultimately prevail as the method of choice for heat exchanger network synthesis (HENS), but computational effort currently limits their application in the case of large problems. The pinch method, on the other hand, offers no guarantee of finding the optimal solution but its application is simple and even large HENS problems can be solved with limited computational effort. (Castier, 2007)

The pinch method offers an efficient route to find heat exchanger networks with minimum use of energy provided by utilities, e. g. cooling water, very low pressure (VLP) steam, etc. It starts with the calculation of targets for minimum utility use and location of the pinch for a specified minimum temperature difference in the heat exchangers. The source and target temperatures of each stream define temperature intervals which are arranged in a so-called problem table. The resulting hot, cold and grand composite curves show where process to process heat integration is possible and how much cooling is necessary from utilities. (Castier, 2007)

For the 1,3-butadiene recovery unit first a basic pinch analysis was carried out. Based on these initial results, a suggestions are made for possible heat integration. The latter are then elaborated in the extended pinch analysis. This analysis forms the basis for the minimum energy design of the heat exchanger network. The methodology followed in this work is based on Douglas (1988). Figure 5 (a) shows the hot and cold composite curve for the optimized 1,3-butadiene recovery unit. As stated previously a temperature approach of 10°C is used. The grand composite curve in Figure 5 (b) shows that indeed internal heat integration is possible, and that utilities remain necessary.
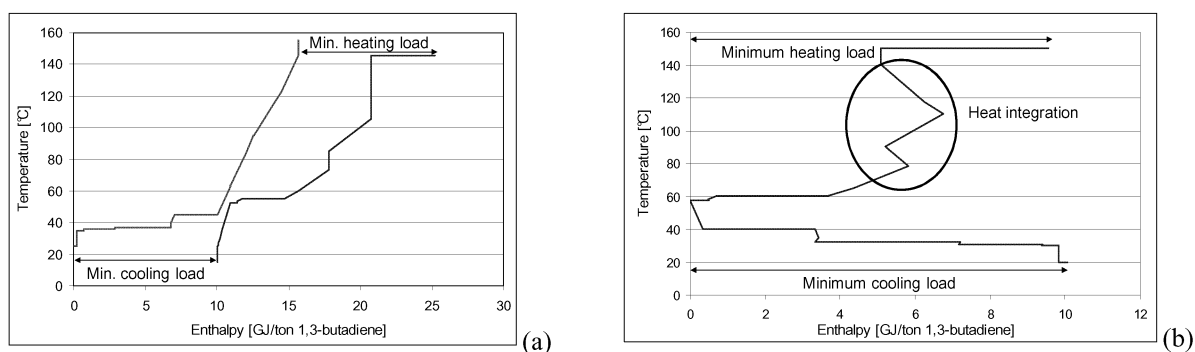

Figure 5: Composite curves: (a) hot and cold composite curve; (b) grand composite curve

Matching of hot and cold streams showed that the energy content of the recycled solvent can be used to partially heat up the feed, the recycle from the second extractive distillation column to the rectifier and the recycle from the degasser to the rectifier. The intercooling in the compressor could be performed by partial heating of the recycle gas from the degasser to the rectifier. No other heat integration is performed due to the fact that most of the cold streams are above the pinch and most of the hot streams are beneath the pinch, making that some matches are insufficient. By matching these streams the net energy requirement of the recovery unit is reduced

with 11 GJ/ton 1,3-butadiene; the hot utilities drop from 14.7 GJ/ton to 9.1 GJ/ton, the cold utilities drop from 15.7 GJ/ton to 10.1 GJ/ton, while the number of heat exchangers increases from 13 to 17.

5. CONCLUSIONS

In the present study a 1,3-butadiene recovery unit is designed with a production capacity of 80 kton/year of polymer grade 1,3-butadiene. For the binary interactions a mix of literature values and values estimated by Aspen were used to obtain simulation results that are in reasonable agreement with industrial findings. Due to the huge amount of recycle streams in the recovery unit numerous convergence issues had to overcome. Using the divided wall column it seems difficult to obtain the design specifications for the present case, and simulations show that certainly no improvement in energy efficiency is expected. The consumption of utilities has been reduced with over 35% by maximizing the internal heat integration via the pinch method.

6. ACKNOWLEDGEMENTS

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