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Internal configurations for a multi-product dividing wall column[☆]

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A B S T R A C T

This paper addresses possibilities and peculiarities associated with establishing the most beneficial internal configuration of a complex dividing wall column (DWC), using as a base case the separation of a multicomponent aromatics mixture into four or five product streams. As expected, the V_{\min} -diagram method proved to be an appropriate tool in such a study, as a means for identifying and assessing promising configurations and at the same time to provide the necessary inputs and reliable initial guesses for detailed simulation-based determination of energy and stage requirements. A new, energy efficient two-top product configuration is introduced that appears to be an interesting option for a four-product DWC.

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1. Introduction

As proven in industrial practice, application of dividing wall columns (DWC), where appropriate, leads to approximately 30% saving in both energy and capital, compared to equivalent conventional distillation sequences for obtaining three high-purity products (Olujić et al., 2009; Asprion and Kaibel, 2010; Dejanović et al., 2010).

In recent papers, Yildirim et al. (2011) and Rong (2011) show a variety of DWC configurations considered suitable for four-product separations. To assess the potential for implementation of four-product DWCs we have taken an industrially relevant case, i.e. an aromatics processing plant as encountered in complex refineries (Dejanović et al., 2011a). For the purposes of our simulation studies, the actual 40-components feed mixture has been reduced to a representative 15-component mixture shown in Table 1. There are four product streams, which are fractions with compositions according to given product specifications.

The design of four-product DWCs has been addressed and encouraging advancements made indicating that a packed DWCs could be arranged as a practical, single-partition wall column shown in Fig. 1, or a thermodynamically optimal, but complex, three-partition walls column, shown schematically in Fig. 2 (Dejanović et al., 2011b). The single-partition wall configuration is generally known as the “Kaibel column”, while the multi-partition wall column, which represents a fully thermally coupled Petlyuk configuration, as shown more clearly for a four-product case in Fig. 3, is sometimes referred to as the “Sargent arrangement” (Cristiansen et al., 1997; Yildirim et al., 2011).

These two configurations are named here “2-4” (Kaibel) and “2-3-4” (Sargent), according to the number of product streams of the columns arranged in series in the flowsheets used for detailed simulation. These two configurations have been simulated and optimized using detailed methods, dimensioned as packed columns and compared on basis of annualized total costs (TAC) using a method thoroughly described elsewhere (Dejanović et al., 2011b).

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Nomenclature

A,B,C,D	products/fractions in order of volatility
B	bottoms flow rate (kmol/h)
C	column
D	distillate flow rate (kmol/h)
F	feed flow rate (kmol/h)
L	liquid flow rate (kmol/h)
N	number of equilibrium stages or theoretical plates
Q	reboiler or condenser duty (kW or MW)
q	feed quality (fraction of the liquid in the feed)
V	vapour flow rate (kmol/h)
w	weight fraction of a component
z	feed composition

Subscripts

A–D	products
B	bottom
C	condenser
R	reboiler
T	top

Acronyms

BRC	benzene rich cut
C1–C33	binary column numbers in Fig. 3
DWC	dividing wall column

It appears that both configurations are highly cost effective compared to a conventional three columns sequence. The “2-4” or Kaibel configuration with seven sections and one vapour split, has been implemented in practice for an undisclosed application in a BASF SE plant as a packed column utilizing J. Montz non-welded wall technology (Olujić et al., 2009).

A detailed inspection of the schematic representation of the “2-3-4” or Sargent configuration (see Fig. 2) shows that this column contains 13 sections and three vapour splits, but as discussed in detail by Dejanović et al. (2011b) it represents an industrially viable option. Such a complex, multipartition four-product DWC could be assembled without great difficulties as structured packing column, by utilizing well established non-welded, self-fixing partition wall technology that provides

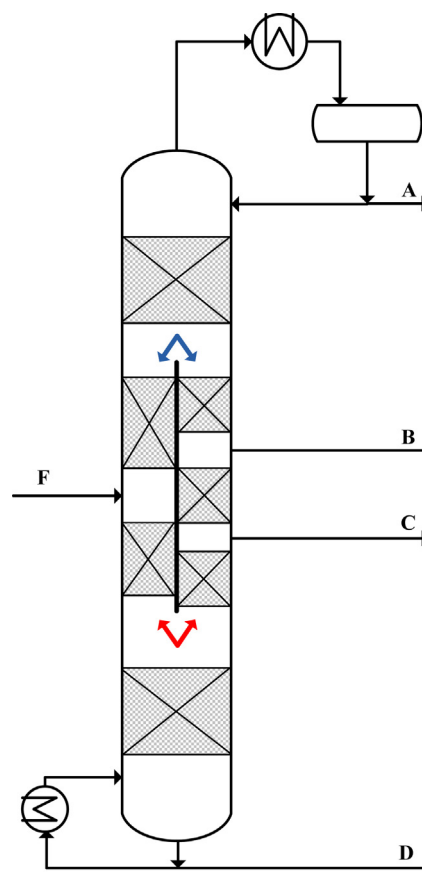


Fig. 1 – Single-partition wall DWC for four-product separation (Kaibel or “2-4” column).

full flexibility in this respect (Kaibel, 2007). Simple and reliable methods for dimensioning conventional, three-product packed DWCs (Dejanović et al., 2011a) have been extended to four-product columns (Olujić et al., 2012).

On the process design side, the main potential drawback lies in the fact that compared to single-partition wall column (“2-4”), the “2-3-4” configuration incorporates three liquid and three vapour splits. While the liquid splits can easily be arranged and manipulated during operation, ensuring a proper vapour split is at present a design challenge. Namely, this needs to be fixed appropriately during column design. Starting from given (fixed) liquid loads and bed heights,

Table 1 – Base case feed and product compositions.

Stream name	Feed (F)	C5-C6 (A)	BRC (B)	Toluene (C)	Heavies (D)
Flow rate [t/h]	31.7	7.44	3.87	8.0	12.41
Mass fractions (rounded)					
n-Butane	0.019	0.086	0	0	0
i-Pentane	0.064	0.284	0	0	0
n-Pentane	0.045	0.201	0	0	0
2-Methylpentane	0.080	0.351	0.010	0	0
N-Hexane	0.043	0.066	0.210	0	0
Benzene	0.086	0.013	0.629	0	0
3-Methylhexane	0.020	0	0.151	0.002	0
Toluene	0.247	0	0	0.984	0.001
Ethylbenzene	0.035	0	0	0.006	0.086
p-Xylene	0.042	0	0	0.003	0.107
m-Xylene	0.122	0	0	0.005	0.307
o-Xylene	0.055	0	0	0	0.140
m-Ethyltoluene	0.047	0	0	0	0.120
1-3-5-Trimethylbenzene	0.077	0	0	0	0.197
1-4-Diethylbenzene	0.017	0	0	0	0.043

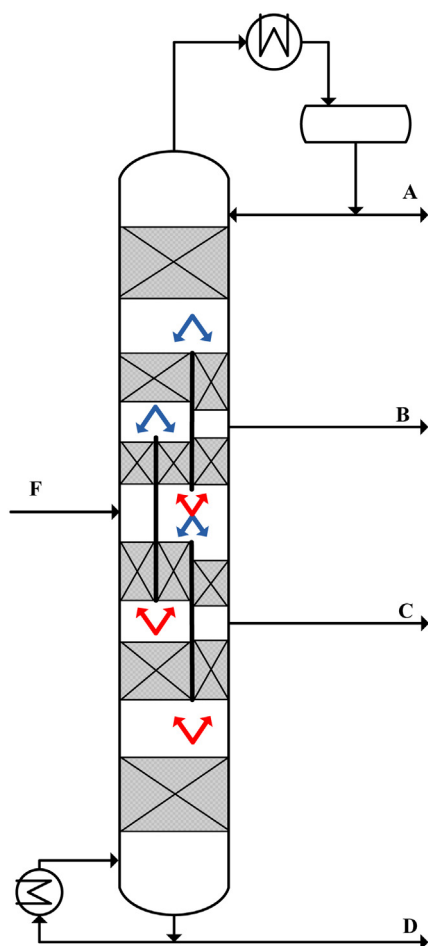


Fig. 2 – A multiple-partition wall DWC for four-product separation (Sargent or “2-3-4” column).

each section in parallel should be arranged to generate the vapour flow resistance that will upon equalization of pressure drop establish a vapour flow throughput complying with the desired liquid to vapour ratio. This could be arranged by careful hydraulic design using existing know-how and technical means (Kaibel, 2007; Dejanović et al., 2011a; Olujić et al., 2012), but operators are generally worried about limited controllability in that respect, regarding potential fluctuations in feed rates and compositions. Indeed, the lack of suitable design procedures, accompanied often by a fear of unstable operation, appears to be a main barrier in this respect.

Control-related aspects of “2-4” (Kaibel) and “2-3-4” (Sargent) configurations have been addressed in separate studies. Dwivedi et al. (2012a) have demonstrated experimentally that in case of a “2-4” configuration, a four-temperature controller structure can handle feed rate disturbances as well as set point changes. In a study concerning basic control structures for the fully thermally coupled, 4-product DWC (“2-3-4” configuration), Dwivedi et al. (2013) have shown that the key is to consider the internal sub-columns and ensure that each sub-column performs its dedicated separation task. During operation the vapour split is normally set by design, and determined by the vapour flow resistances in the parallel flow paths. An experimental study by Dwivedi et al. (2012b) shows that it is feasible to implement active vapour split manipulation. This may be beneficial in order to obtain full energy savings for a larger range of feed composition variations since the optimal splits depend on the feed properties.

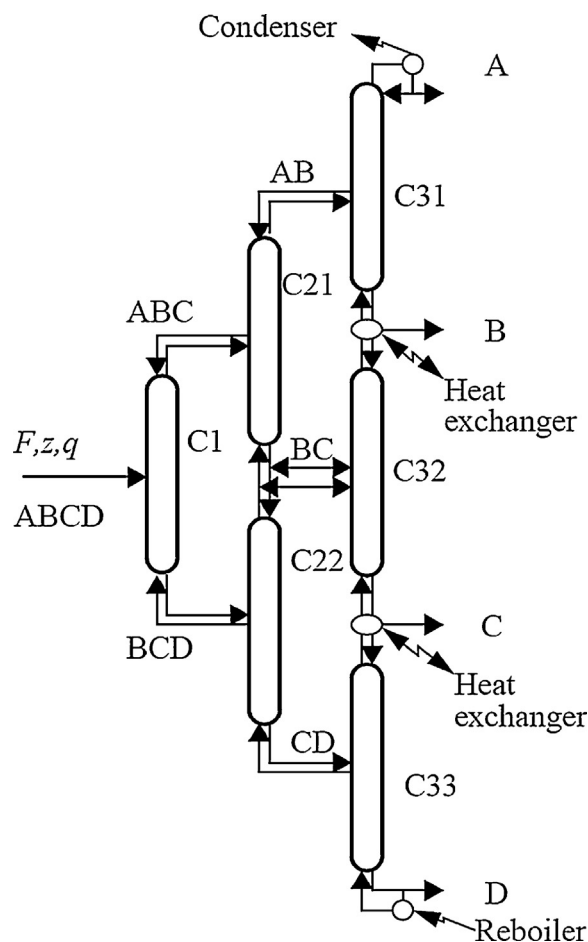


Fig. 3 – Fully thermally coupled Petlyuk sequence for separation of a four component mixture into pure components, including two side heat exchangers allowing additional heat coupling flexibility.

These and other simulation studies have shown that so called V_{\min} -diagram method (Halvorsen and Skogestad, 2003, 2011) is a simple and robust practical means that can be used to identify and quantify accordingly internal configuration of a DWC. In addition, it provides reliable data for initialization and effective execution of detailed energy and stage requirement calculations, using facilities available in a commercial software package (Dejanović et al., 2011b). Detailed simulations indicate that the energy saving potential of the complex “2-3-4” (Sargent) configuration is such that it is certainly worth to consider its practical implementation. In the present case study, the energy saving is about 20% (or 1MW) compared to the Kaibel configuration.

Considering the fact that arranging and controlling three vapour splits appears to be a major design and operation concern, related uncertainties could be lessened significantly if the number of required vapour splits could be reduced. Again, a V_{\min} -diagram based analysis proves to be highly revealing, as will be shown in the following by suggesting more practical internal configurations for a four-product DWC and by introducing a new, two overhead products configuration, with two separate condensers, that allows additional flexibility in the control of vapour splits. In addition to this, a five-product DWC is considered, just to demonstrate the versatility and usability of the V_{\min} -diagram method.

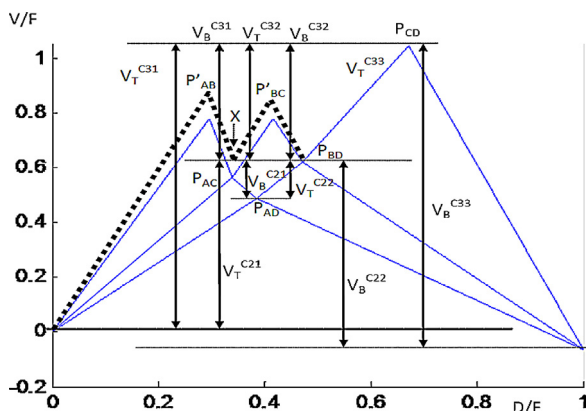


Fig. 4 – V_{\min} -diagram (solid lines) corresponding to Petlyuk sequence shown in Fig. 3. Dotted lines represent a modified configuration described in the text.

2. Basic 4-product configurations

The V_{\min} -diagram can be constructed in a straightforward way based on feed properties only and gives the detailed optimal set of internal flow rates for the fully extended Petlyuk or Sargent (“2-3-4”) arrangement in Fig. 2. An equivalent thermodynamic representation using a sequence of binary columns for a four-product separation is shown in Fig. 3, where the two side heat exchangers are not necessary but provide, as it will be shown later, additional flexibility regarding potential configuration of a DWC.

Fig. 4 shows the V_{\min} -diagram for the four-product case considered in this study. The total energy requirement corresponds to the (V/F) ratio of the most difficult among binary separations. In the present case, the most demanding separation appears to be the separation between components C and D, which is represented by the peak P_{CD} . The base diagram shown in solid lines corresponds to the fully extended Petlyuk arrangement (“2-3-4” configuration) while the dotted lines show another arrangement discussed in detail later.

The diagram is constructed by calculating the values of V/F and D/F of characteristic points in the diagram (peaks and saddles), representing cuts of desired recoveries between any possible pair of key components in the feed mixture, which occur in various sections of a DWC. One should note that similar to other short-cut distillation methods, the construction of a V_{\min} -diagram using analytical expressions is based on assumptions of constant relative volatilities, constant molar overflows and infinite number of stages. The analytic expressions are based on the well-known minimum reflux Underwood equations, and the data required to initiate the calculations are molar fractions of the components in the feed, K -values of the components at feed conditions (pressure and temperature) and the liquid fraction of the feed. In the case of multicomponent mixtures the lines representing separation between key-components in each product are shown, so the method is not limited with respect to the number of components and product distribution. In the present case study, the 15-component feed mixture in Table 1 has been reduced to five key-components, according to given product specifications (Olujić et al., 2012).

The V_{\min} -diagram can also be obtained for real mixtures by performing a series of binary distillation simulations in a commercial process simulator, using the same feed mixture every time, but changing the key components and recoveries using

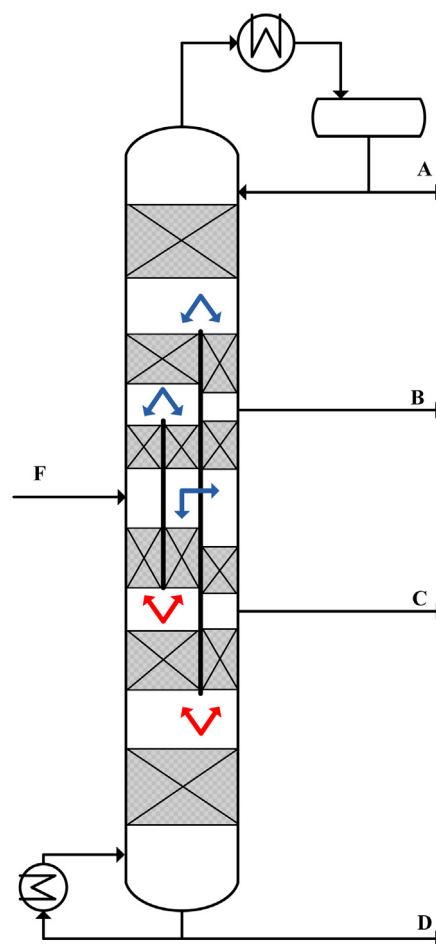


Fig. 5 – Schematic illustration of “simplified 2-3-4” configuration.

approximately four times the minimum number of stages, as calculated by Fenske equation.

Most importantly, the V_{\min} -diagram provides directly information related to the internal configuration of a DWC with all individual liquid and vapour flow rates at minimum reflux

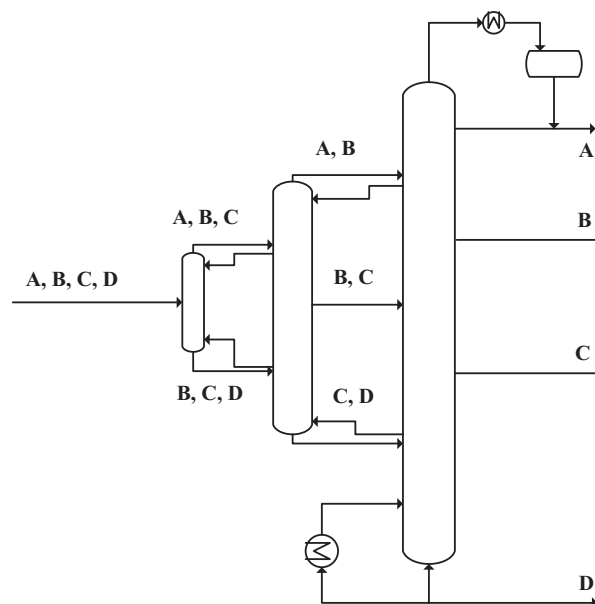


Fig. 6 – The flow-sheet used for detailed simulation “simplified 2-3-4” configuration.

condition, as well as required liquid and vapour splits. The corresponding numbers are excellent initial guesses for detailed (rigorous) calculations that are required to determine stage and energy (reflux) requirements for a given situation. This, however, is not straightforward, because it requires assembling an appropriate flowsheet using the facilities available in commercial software packages. The flowsheets used to simulate “2-4” and “2-3-4” configurations in ChemCAD can be found elsewhere (Dejanović et al., 2011b).

For the design case considered here, detailed calculations give a reboiler duty of 4.81 MW for the fully thermally coupled “2-3-4” configuration. It corresponds to the most demanding separation between components C and D (peak P_{CD}) and covers the needs of all other separations, i.e. those involving neighbouring components A and B and B and C, represented by peaks P_{AB} and P_{BC} , and less demanding separations between A and C and A and D, represented by valleys (knots) P_{AC} and P_{BD} , respectively. The lowest point P_{AD} corresponds to easiest (sloppy) separation between lightest and heaviest component, i.e. A and D.

A closer inspection of the given situation indicates that there may be some freedom, i.e. possibility for rearranging the middle section, by either changing prefractionator

operation settings or component splits in the bottom or upper parts. As indicated for one of these cases by the dotted line in the V_{\min} -diagram in Fig. 4, possible modifications of internal configuration are characterized by a shift in heights of peaks, and the upper limit in this respect is the level of the highest peak setting the maximum boil-up requirement (P_{CD} in present case). This will be elaborated in greater detail in what follows. In addition to this and to demonstrate versatility of V_{\min} -diagram and its usability as a DWC assessment tool, our four-product DWC has been rearranged into a five-product DWC, by incorporating the separation of benzene rich stream into benzene and 3-methylhexane.

3. Alternative 4-product DWC configurations

3.1. A simplified “2-3-4” 4-product DWC

The fully thermally coupled “2-3-4” configuration, which utilizes three vapour splits, could be simplified by separating the main column side from the central (middle) section by a continuous partition wall, as shown schematically in Fig. 5,

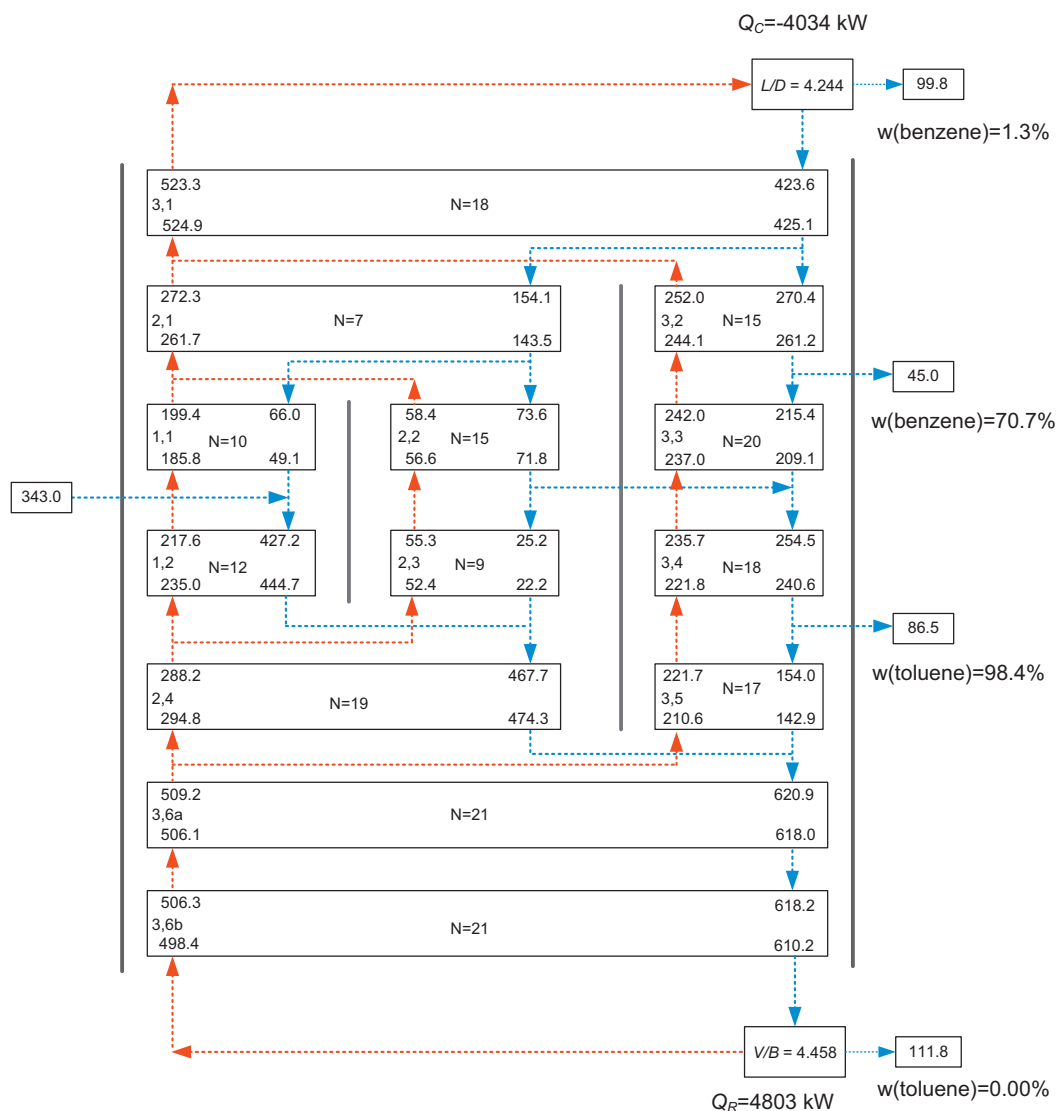


Fig. 7 – Mass balance of “simplified 2-3-4” configuration, with all internal molar liquid and vapour flow rates, and stage requirement per section according to detailed simulation.

allowing only the required flow of liquid to enter the main column section (sub-column C32). This means introduction of a larger vapour load in the upper part of the middle section (sub-column C21), which should effectively be that of the bottom of the sub-column C22. This can be achieved by shifting the operating point of C21 (point P_{AC} in the V_{min} -diagram, representing the A/C split), until it reaches the same height as the operating point of C22 (point P_{BD} in the V_{min} -diagram, representing the B/D split). This also lifts operating points P_{AB} and P_{BC} , increasing vapour demand in sub-columns C31 and C32 to the level indicated by the dotted line in Fig. 4. Since new operating points are still lower than the highest point (peak) in the diagram, e.g. P_{CD} , the required reboiler duty will remain unaffected.

The flow-sheet of this configuration used for rigorous simulation purposes is shown in Fig. 6. The reboiler duty is the same (4.81 MW) as in the full “2-3-4” (Sargent) case, and the number of stages was gradually reduced and the material flows in C21 and C22 adjusted, until the desired product specifications were achieved. The results, i.e. appropriate internal configuration and molar liquid and vapour flows at the top and bottom of each packed bed, are shown in Fig. 7. The number of required equilibrium stages remained equal to that of the original “2-3-4” configuration, i.e., 202.

The simplified “2-3-4” configuration, referred to as “s-2-3-4”, though containing the same number of sections, requires one vapour split less, which may be considered as a significant advantage from both the design and operating point of view. Due to the shift in vapour and liquid flows in the upper part of middle and main column section, the cross-sectional area of the middle section increases and that on the main column side decreases accordingly.

3.2. A practical 4-product DWC

The following configuration is based on a change in the prefractionator operation point, by moving the split between B and C to C and D, to ensure a full recovery of B in the distillate stream. This is visualized by the dotted lines in V_{min} -diagram in Fig. 4, simply by moving the prefractionator operating point, P_{AD} , upwardly to the right until it overlaps with P_{BD} . With this, the net distillate flow from sub-column C22 becomes zero. Consequently, this leads to increased prefractionator load, however the overall vapour flow rate remains the same, because peaks P_{AB} and P_{BC} are considerably lower than P_{CD} . Fig. 8 shows schematically the resulting internal configuration.

Practically, this means that sub-column C22 (see Fig. 3) is not necessary and can be removed as indicated in the flow-sheet shown in Fig. 9, which served as basis for rigorous simulation of this configuration. The results of the rigorous simulations are summarized graphically in Fig. 10. Interestingly, the total stage requirement of this configuration is significantly lower, i.e. 174, and approaching that of Kaibel column, i.e. “2-4” configuration (169 stages).

This arrangement, referred to as “2-2-4” configuration, is similar, but it is simpler than the one known in the literature as the “Agrawal arrangement” (Cristiansen et al., 1997; Yildirim et al., 2011). Most importantly, this configuration reduces the number of vapour and liquid splits to two and can be arranged in 11 sections. Although the number of required stages is much lower than with other configurations this will not result in a reduction in packing volume and column height. The reason is that the same space is now a part of the extended, joint

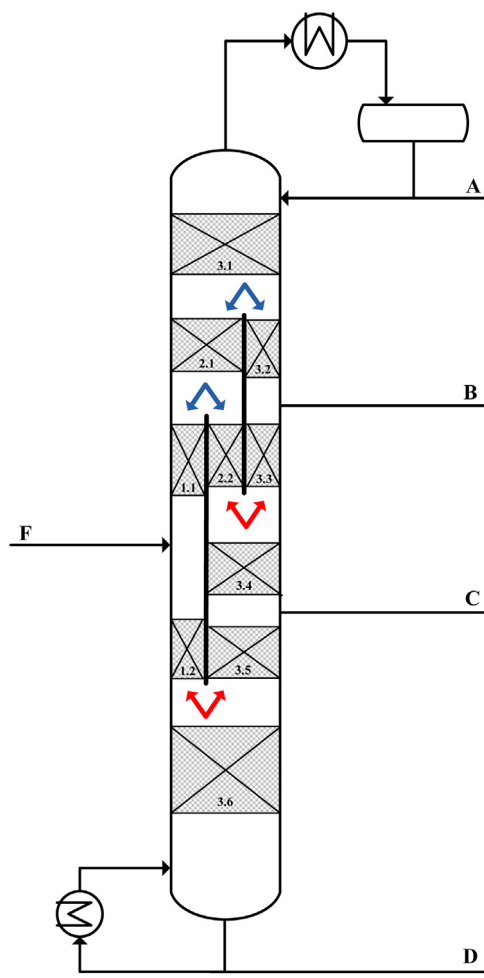


Fig. 8 – Schematic illustration of “2-2-4” configuration.

bottom section of the middle and main column, while the number of stages on main column side remains the same. On the other hand, the internal vapour and liquid flow rates on critical places are similar, which means that section diameters will remain the same. As illustrated in greater detail elsewhere (Olujić et al., 2012), for this configuration with 11 sections and

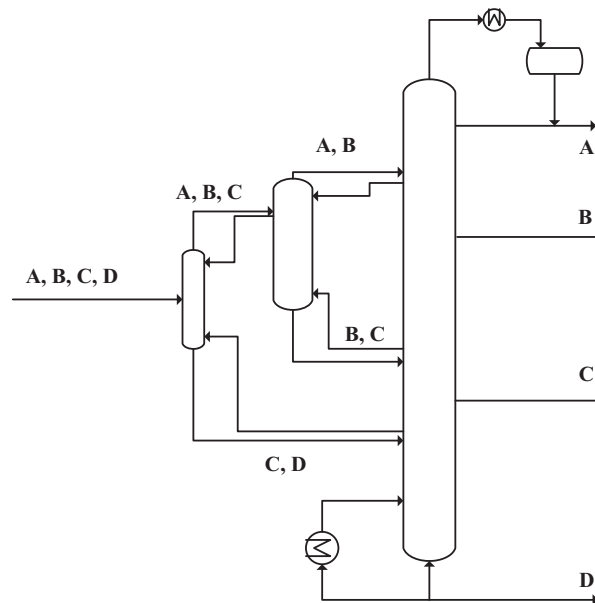


Fig. 9 – Flow-sheet used for detailed simulation of “2-2-4” configuration.

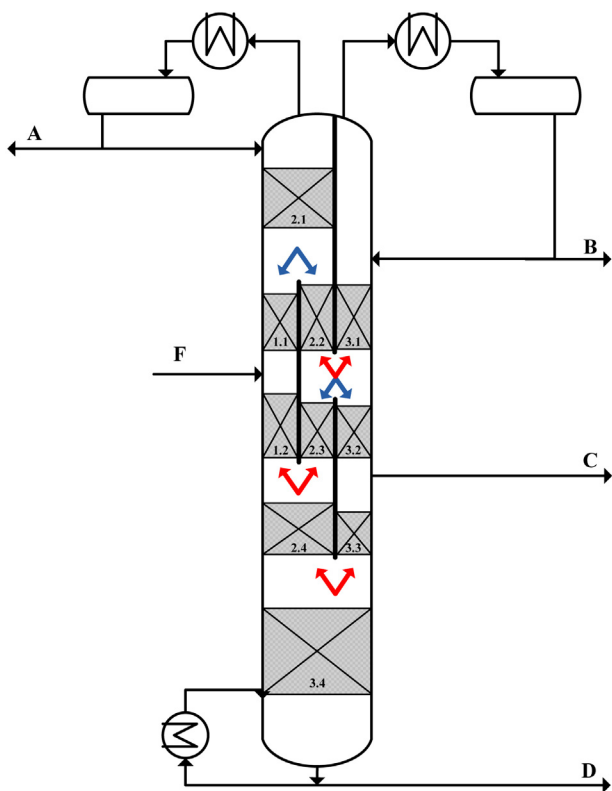


Fig. 11 – Schematic illustration of “2-3-3” configuration.

The flowsheet used for detailed simulation of this configuration is shown in Fig. 12, and the estimated stage requirement and individual molar liquid and vapour flows for each section are shown in Fig. 13. This arrangement, referred to as the “2-3-3” configuration, includes 10 sections with in total 202 stages distributed between the prefractionator (2 sections), middle

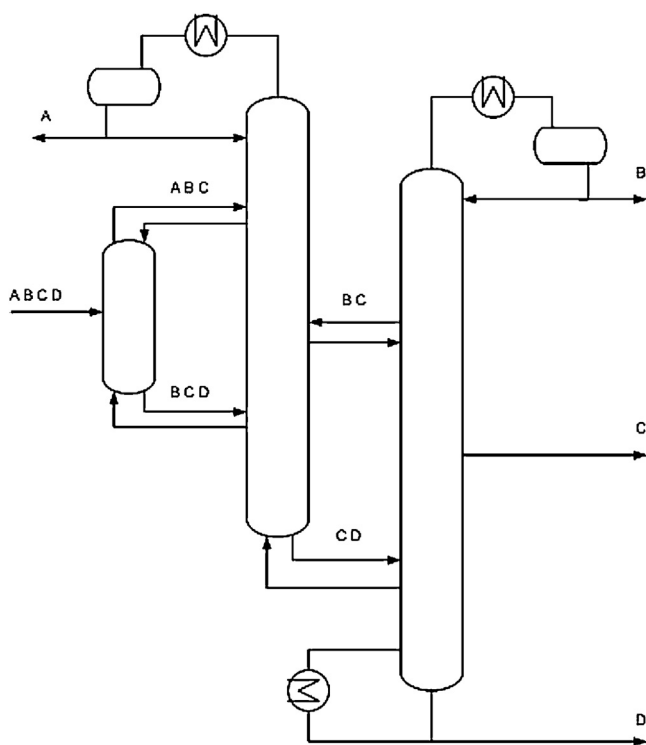


Fig. 12 – Flow-sheet used for detailed simulation of “2-3-3” configuration.

column (4 sections) and main column (4 sections). A comparison with the basic “2-3-4” configuration shown in Fig. 2 indicates a certain shift in the number of stages required per section, while both liquid and vapour loads of the partitioned part of the middle sections are much larger. The latter implies that the cross-sectional areas of the middle section increases at the cost of that of the main column section.

Interestingly, the liquid and vapour splits in this part of the main column are oriented in opposite direction, i.e. liquid from the middle section feeds the lower part of the main column section, while the vapour ascending from the lower part of the main column section is partly fed to the upper part of the middle section. In total, this configuration requires two liquid and three vapour splits.

Although the need for an additional condenser suggests increased capital cost, this may be compensated by a significantly reduced total shell height. This is because in this configuration the stages are more evenly distributed between the middle- and main-column sections, with a maximum height equivalent to 116 stages, as required for the middle section, while the shell of the “2-2-4” configuration must accommodate 130 stages, as required for the main column section. Since we have equal reboiler duty, the boil-up and shell diameter should remain the same. The cost effectiveness of this configuration will be evaluated upon completing the dimensioning of the column, which is the subject of a forthcoming study.

It is interesting to note that in the present case study, where the minimum vapour requirements for the A/B and B/C splits are considerably lower than that for the C/D split, the configuration with the partitioned top of the column does not necessary need a higher energy demand, as suggested elsewhere (Kaibel, 2007). An important benefit of the “2-3-3” configuration is that the upper section vapour split can be manipulated to a certain extent by adjusting the condenser duty. This allows some flexibility in handling fluctuations in feed composition. Other configurations are more limited in this respect. In general, feed composition fluctuations can be compensated, but to a lesser extent, by adjusting the feed quality (q -value). This, however, depends on the case and should be considered and evaluated properly at the conceptual design phase. This is also the case for more detailed controllability analysis of the simplified configurations. The general guidelines for controlling internal sections can most likely be based on the results for the full “2-3-4” configuration (Dwivedi et al., 2013). As the simplified internal configurations have fewer sections and manipulative inputs, less complexity of the control structure is also expected. The two external condensers of the “2-3-3” configuration also give the opportunity to adjust an internal vapour split. But as is the case with distillation columns in general, the purity specifications and the expected feed rate and composition disturbances will be important factors in control structure design.

4. A 5-product DWC

For the purpose of demonstrating a 5-product DWC design, the benzene-rich stream is assumed to be further separated into benzene and 3-methyl hexane rich products. This is shown as streams B1 and B2 in Fig. 14. The corresponding V_{min} -diagram (see Fig. 15) shows that the characteristic peak and corresponding heat requirement is below the highest one, indicating that this additional separation can be performed

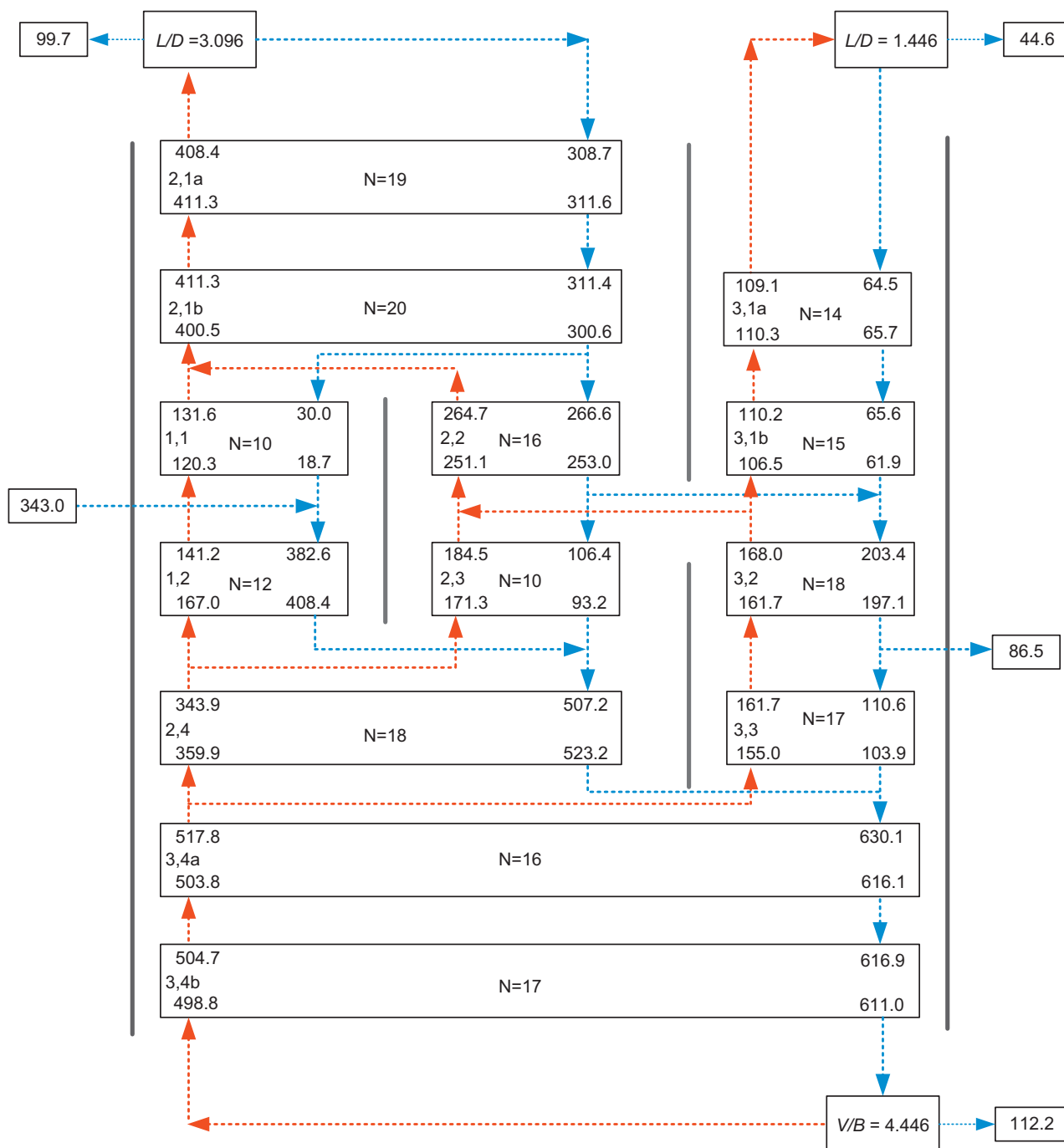


Fig. 13 – Mass balance of “2-3-3” configuration, with all internal molar liquid and vapour flow rates, and stage requirement per section according to detailed simulation.

without adding energy. This is appealing; however it is accompanied by an increased complexity of the design, because it requires another set of sub-columns in parallel, increasing the number of sections to 19. Fig. 16 shows the complex flow-sheet used for detailed simulation of this configuration.

Results of detailed simulations are shown in Fig. 17, where stage requirements and internal liquid and vapour flow rates are shown for each section of the column. We see that compared to the 4-product DWC alternatives, this column contains additional 53 stages in the main column section. This is difficult to accommodate in one shell, because the distribution of stages is highly unsymmetrical, with much more stages required in the main column section, which means a lot of empty space on the prefractionator column side, as well as in the two middle sections. Also, four sections in parallel in

the partitioned part of the column are required. Since these are separated by continuous partition walls, three liquid and three vapour splits are required. All this appears unfavourable and suggests that instead an external column, in addition to a 4-product DWC (see Fig. 16), could be a practical solution.

Finally, it should be mentioned here that the V_{\min} -diagram has been used recently by Kiss et al. (2013) as a tool for evaluation of a five-product aromatics separation using various sequences of 3-product DWC, conventional 2-product columns and 4-product Kaibel-columns.

5. Concluding remarks

To achieve the minimum energy requirement, four-product DWCs require a complex internal configuration with a

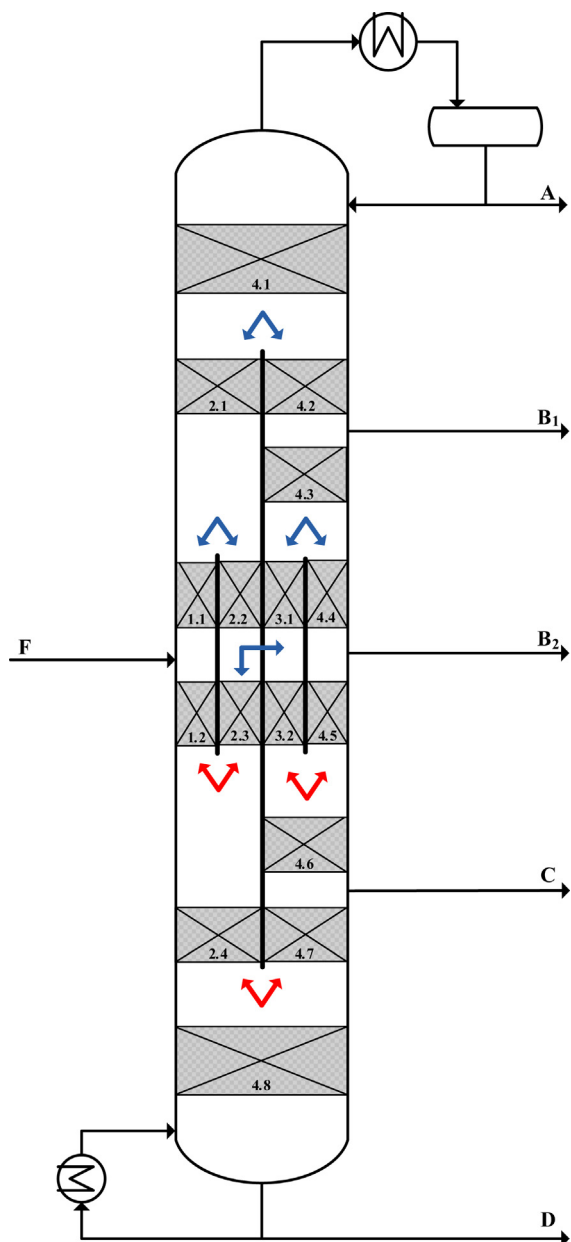


Fig. 14 – Schematic illustration of a 5-product DWC (“2-3-4-1” configuration).

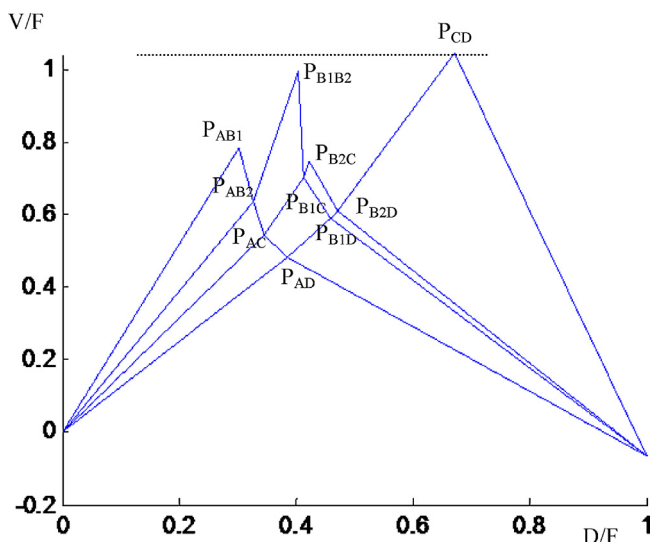


Fig. 15 – Simplified version of V_{min} -diagram of a 5-product “2-3-4-1” configuration.

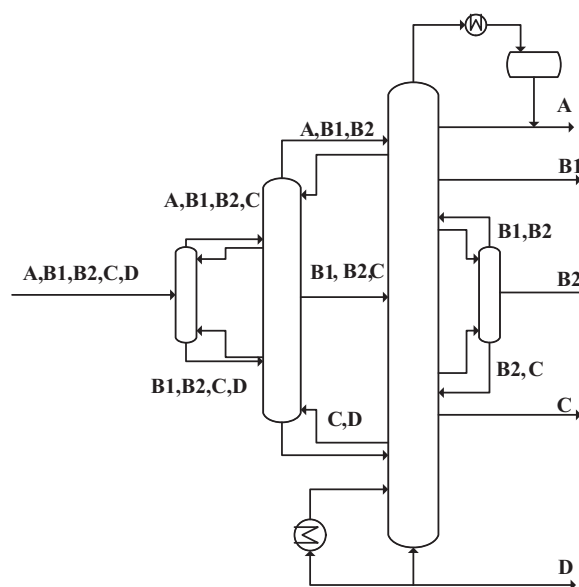


Fig. 16 – The flow-sheet used for detailed simulation of the 5-product configuration.

middle or central section in between the prefractionator and the main column. Depending on the chosen arrangement, two or more partition walls may be needed.

The assessment of alternative configurations has been carried out using the V_{min} -diagram method. In addition to the conventional configuration, representing a fully thermally coupled Petlyuk case with three vapour splits, two simpler configurations emerged, each with two vapour splits. The simplified configurations were simulated and optimized by detailed calculations using results of V_{min} -diagram as initial guesses. The results show that the complexity of the internal configuration of a minimum-energy 4-product DWC can be reduced to a level that encourages practical implementation. The V_{min} -diagram also indicates that the minimum reboiler duty remains the same also for the simplified configurations for the given feed case. This is confirmed by the rigorous simulations.

The stage and reflux requirements of all configurations are summarized in Table 2. Alternatives for four-product separation, i.e. “s-2-3-4”, “2-2-4” and “2-3-3”, require one vapour and/or liquid split less than the “2-3-4” configuration with three vapour and three liquid splits. Since the former two require only two vapour splits, these configurations are considered to be more practical from implementation point of view than those with three vapour splits. Because of the additional constructional and installation advantages evaluated in detail elsewhere (Olujić et al., 2012), the “2-2-4” configuration is suggested for practical implementation. Two-overhead-products configuration (“2-3-3”) requires a second condenser, and a lower stage number along the vertical axis indicates that this column will require a somewhat lower shell height.

Regarding the base case considered in present study, the internal configuration of the two-partition walls 4-product DWC shown in Fig. 8 appears to be the simplest and most practical one, which, if implemented, could contribute to a significant increase in profitability of aromatics processing plants.

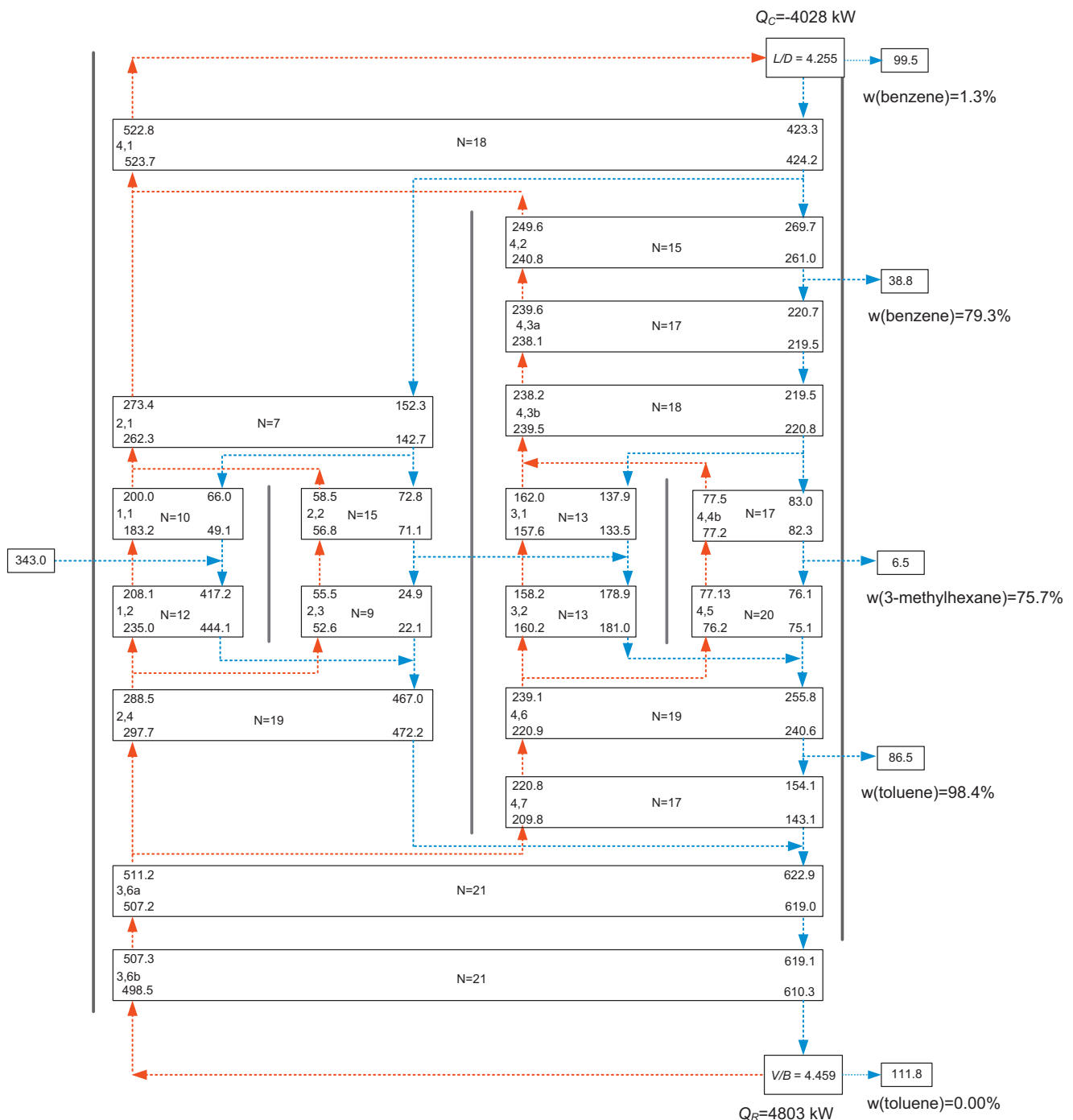


Fig. 17 – Mass balance of 5-product configuration, with all internal molar liquid and vapour flow rates, and stage requirement per section according to detailed simulation.

Table 2 – Energy and stage requirement of five 4-product and a 5-product configurations.

DWC configuration	“2-4”	“2-3-4”	“s-2-3-4”	“2-2-4”	“2-3-3”	“2-3-4-1”
Reboiler duty (MW)	5.82	4.81	4.81	4.81	4.81	4.81
Number of eq. stages	169	202	202	174	202	291
Stage count determining shell height	129	130	130	130	116	183

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