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Chemical Engineering Research and Design

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Designing four-product dividing wall columns for separation of a multicomponent aromatics mixture

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ABSTRACT

Preliminary evaluations using a simple but reliable short-cut method indicated that a 15 component aromatics mixture can be separated very efficiently into four fractions according to the given product specifications employing either a single or a multiple partition wall dividing wall column (DWC). The obtained results have been used to initiate rigorous simulations, to determine the number of stages required in different sections, as well as to obtain internal flows of vapour and liquid necessary for dimensioning and adequate cost estimation for two design alternatives. Based on the comparison of total annualised costs it appears that a multi-partition wall configuration that maximizes energy efficiency is a more attractive option for implementation in aromatics processing plants than more practical single partition wall configuration.

Keywords: Distillation; Energy saving; Dividing wall column; Thermal coupling

1. Introduction

Separation by distillation is responsible for a large fraction of immense amount of energy consumed in process industries. Therefore distillation operations became a major concern within sustainability challenge, i.e. a primary target of energy saving efforts in industrially developed countries (Humphrey and Keller, 1997). Being by far the most widely used separation process in industrial practice, utilizing largest scale equipment, distillation is both most energy and most capital intensive process technology. Driven by global industrial growth it tends to grow in both number and size of applications (Olujić et al., 2009). Hence the present day challenge is to design distillation systems that at the same time are sustainable and economically feasible.

Most promising in this respect are so-called dividing wall columns (DWC). DWC is in essence a fully thermally coupled distillation sequence, with one condenser and one reboiler regardless of the number of products, packed into a single shell, by means of one or more longitudinal partition walls. This configuration minimizes entropy of mixing formation simply by avoiding effectively internal re-mixing of streams. Its special feature is that it is the only known large scale processing intensification example, where both capital and energy expenses can be reduced, with additional benefit of reduction of required installation space.

So far, only single-partition wall DWCs have found wide application in practice (Olujić et al., 2009; Asprion and Kaibel, 2010; Dejanović et al., 2010a). However, by adopting non-welded partition wall technology it became possible, not only to expand the application window for three products columns but also to think of implementing four and more products separations in one DWC. This implies installation of several partition walls in off-centre positions and in parallel, which however is a challenge for dimensioning because a proper distribution of vapour immediately below the partition wall

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Received 1 November 2010; Received in revised form 12 January 2011; Accepted 22 January 2011

doi:10.1016/j.cherd.2011.01.016

Table 1 – Feed and product streams base case data.

Stream	Property				
	Platformate	C5-C6	BRC	Toluene	Heavies
Temperature (°C)	37.0	40.0	115.3	111.1	163.6
Pressure (bar)	3.01	2.70	3.17	1.01	1.56
Flow rate (kmol/h)	343.0	97.8	47.1	86.5	111.6
Flow rate (t/h)	31.73	7.16	4.16	7.86	15.55
Mass fraction					
n-Butane	0.019	0.086	–	–	–
i-Pentane	0.064	0.284	–	–	–
n-Pentane	0.045	0.201	–	–	–
2-Methylpentane	0.080	0.351	0.010	–	–
n-Hexane	0.043	0.066	0.210	–	–
Benzene	0.086	0.013	0.629	–	–
3-Metylhexane	0.020	–	0.151	0.002	–
Toluene	0.247	–	–	0.984	0.001
Ethylbenzene	0.035	–	–	0.006	0.086
p-Xylene	0.042	–	–	0.003	0.107
m-Xylene	0.122	–	–	0.005	0.307
o-Xylene	0.055	–	–	–	0.140
m-Ethyltoluene	0.047	–	–	–	0.120
1-3-5-Trimethylbenzene	0.077	–	–	–	0.197
1-4-Diethylbenzene	0.017	–	–	–	0.043

has to be ensured during the design phase by arranging the pressure drop of each partitioned section accordingly.

In this paper, we show a comparison of a properly dimensioned single-partition wall column for obtaining four products with a three-partition wall column. As indicated in conceptual design stage and confirmed by rigorous simulations in present work, the latter maximizes the energy saving gain with respect to conventional three columns sequence. However such a complex internal DWC configuration has not been attempted yet in industrial practice. As it will be demonstrated later on, in present case a multiple-partition-wall DWC appears to be an industrially viable option.

2. Base case design

The existing aromatics plant in a petroleum refinery is used to remove as much benzene as possible, as a heart cut, from the platforming process reactor effluent stream (31.73 t/h, 3.01 bar, 37 °C, slightly under-cooled liquid, i.e. $q = 1.064$) that contains 40 components. For the purposes of this study, these have been lumped together accordingly into a representative 15 components mixture. The separation by distillation is performed in a conventional two-column direct sequence, producing C_5–C_6 gasoline with less than 1.5 mass% benzene, benzene rich cut (BRC) with 68 mass% benzene content, and heavy platformate, consisting mostly of toluene and heavier aromatics, with less than 0.5 mass% benzene. This three-product sequence was successfully simulated using ChemCAD (Dejanović et al., 2010b).

In order to acquire a base-case design for a four-product sequence, a third column was added to effect separation of a toluene rich (>98 mass%) stream from ethylbenzene and heavier components. Thus the separation is performed according to the arrangement shown in Fig. 1, which is regarding energy requirement similar to equivalent direct sequence. It can be easily implemented, simply by adding the 3rd column, without changing the operation of the existing sequence. Product stream compositions obtained by simulation of this three-column configuration are shown in Table 1.

3. 4-p DWC modelling and evaluation

3.1. *Alternative 4-p DWC configurations*

Two feasible options for a 4-product dividing wall column (4-p DWC) are shown schematically in Fig. 2a and b. Fig. 2a shows a so-called Kaibel configuration (Kaibel, 1987; Olujić et al., 2009) employing one partition wall, and Fig. 2b shows a so called fully extended Petlyuk configuration, that employs multiple partitions walls. The former implies having two and the latter one three sections in parallel. According to various simulations studies (see Dejanović et al., 2010a), the former enables

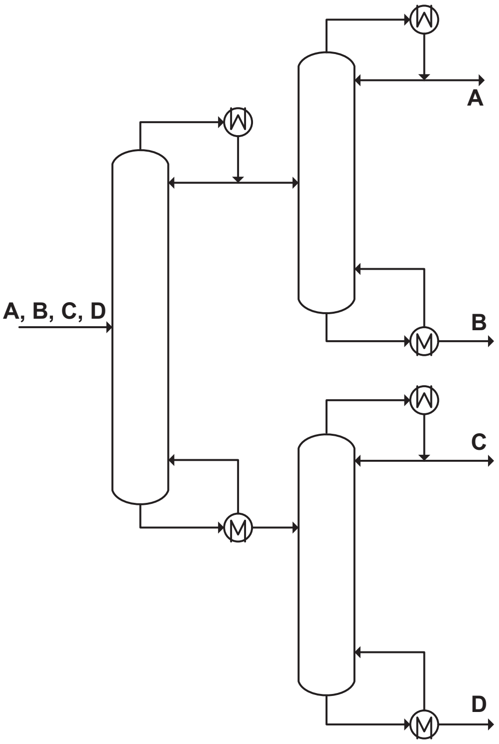
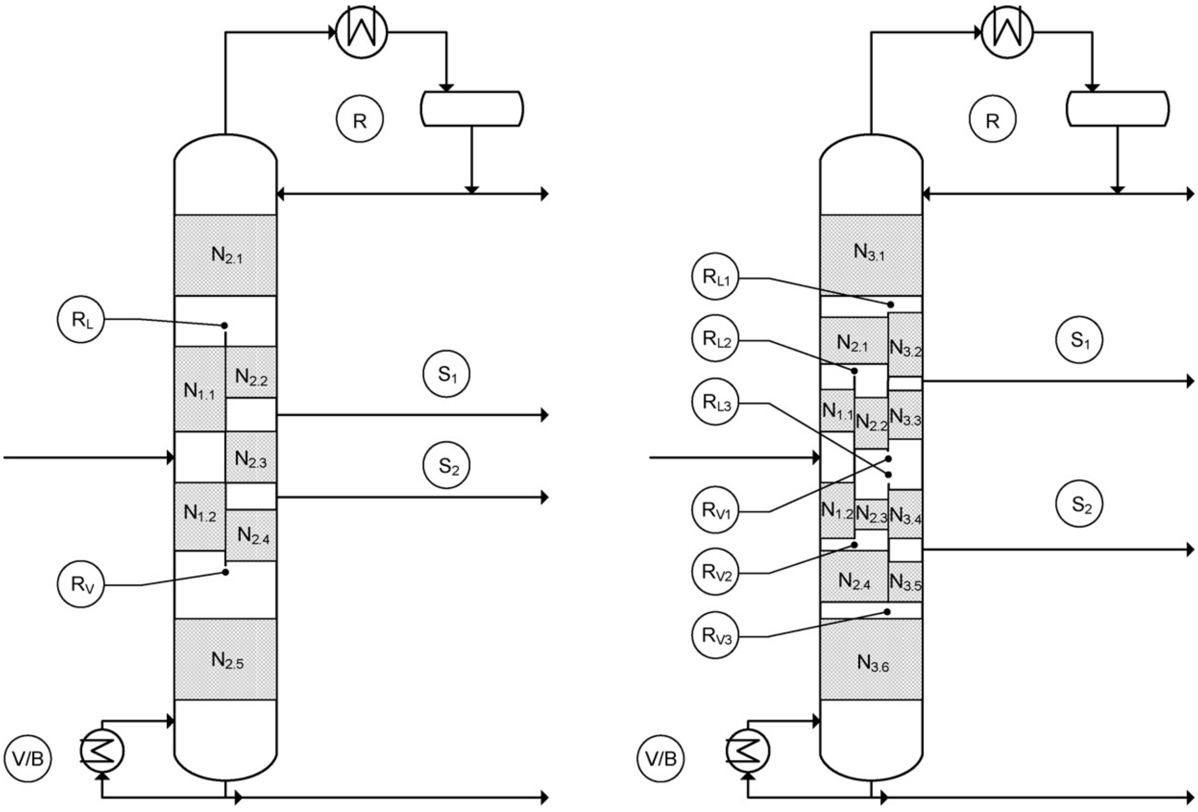


Fig. 1 – Base case configuration.



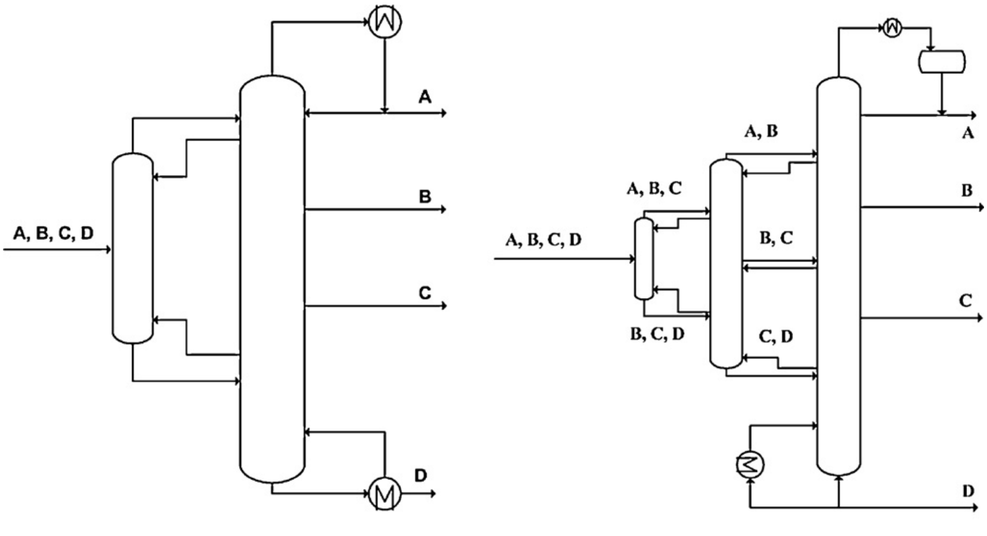
“2-4” “2-3-4”

Fig. 2 – Schematic illustration of two alternative four-product DWCs: Kaibel column – (“2-4”) and the fully extended Petlyuk (“2-3-4”) configurations.

a significant energy saving with respect to conventional configuration, which however is well below that achievable with a fully extended counterpart.

However, the only known application so far of a 4-p DWC is the simpler, Kaibel type column, with one partition wall, with longitudinal sections in off-centre position (see Olujić et al., 2009), which was adopted because of practical reasons, i.e. its simpler design, construction and operation. The complexity, i.e. design, operation and control related uncertainties seems to be the main reason that multiple partition wall configurations, which maximize energy saving, have not yet been attempted in industrial practice.

An objective of this paper is to demonstrate that design of internal configuration of a complex DWC is something that can be done with certainty, and that column dimensioning can be performed with some confidence for applications utilising columns equipped with structured packings, using the public domain knowledge. Namely, well established and highly



“2-4” configuration “2-3-4” configuration

Fig. 3 – Simple column sequences used for detailed simulation of a DWC.

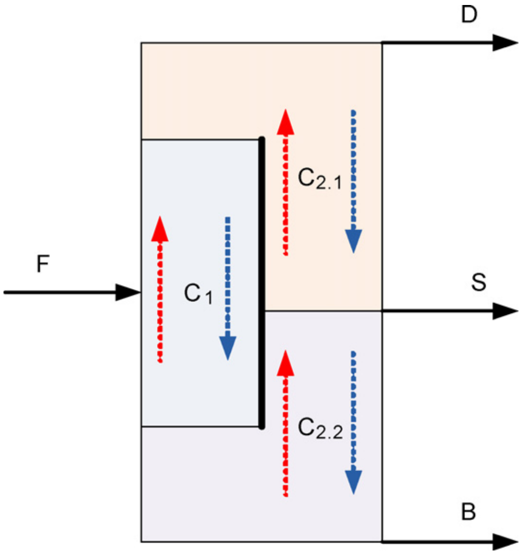


Fig. 4 – Partitioned part of a DWC represented as a prefractionator column coupled with two two-product columns, resembling base case configuration shown in Fig. 1.

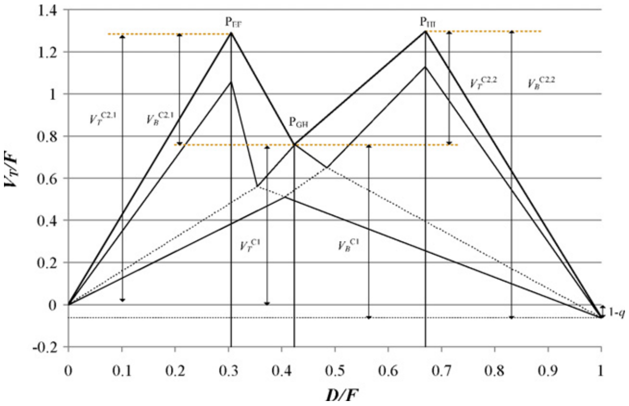


Fig. 5 – V-min diagram for “2-4” configuration.

practical non-welded partition wall technology, described in greater detail elsewhere (Kaibel et al., 2007; Olujić et al., 2009; Dejanović et al., 2010a), allows assembling multiple partition wall configurations without additional difficulties.

Table 2 – Calculation initialisation data required by V-min diagram method.

Tag	Component	z_i	K_i	Product
A	n-Butane	0.0308	6.2768	D
B	i-Pentane	0.0821	3.3869	D
C	n-Pentane	0.0581	2.8330	D
D	2-Methylpentane	0.0863	1.6298	D
E	n-Hexane	0.0456	1.3261	D
F	Benzene	0.1013	0.9417	S_1
G	3-Metylhexane	0.0187	0.7347	S_1
H	Toluene	0.2484	0.4154	S_2
I	Ethylbenzene	0.0306	0.2032	B
J	p-Xylene	0.0370	0.1888	B
K	m-Xylene	0.1062	0.1851	B
L	o-Xylene	0.0477	0.1637	B
M	m-Ethyltoluene	0.0363	0.0962	B
N	1-3-5-Trimethylbenzene	0.0595	0.0841	B
O	1-4-Diethylbenzene	0.0114	0.0478	B

$q = 1.0641$ (slightly sub-cooled feed!).

Two alternative configurations can be simulated using facilities available in commercial software packages by employing corresponding thermodynamically equivalent sequences of simple columns. These are shown schematically in Fig. 3a and b, respectively. In case of “2-4” configuration, a prefractionator column delivers two products as feed streams to a four product column, and the “2-3-4” configuration consists of a two products prefractionator feeding a middle column delivering three product streams as feeds for the main, four products column. According to Fig. 2a and b, respectively, former requires 13, while the latter requires 22 parameters to be fully defined, i.e. to allow performance simulation using models suitable for this purpose. This implies dealing with computational difficulties, which however could be avoided by employing a robust, design-oriented short-cut method to generate reliable estimates of governing variables for initialization of detailed calculations.

3.2. *Short-cut modelling approach*

According to a most recent state of the art review (Dejanović et al., 2010a), the so called V-min diagram method, introduced and elaborated in detail in recent publications by Halvorsen and Skogestad (2003a,b,c) represents a universal engineering

Table 3 – Characteristic points of the V-min diagram shown in Fig. 5.

Section	Split	Specified		Calculated			
		Recoveries		V_T/F	D/F	N	N_f
C1	$P_{G/H}$	$r(I,D) = 0.01$	$r(E,B) = 0.01$	0.76	0.4252	75	38
C2.1	$P_{E/F}$	$r(H,D) = 0.05$	$r(E,B) = 0.05$	1.28	0.3057	100	50
C2.2	$P_{H/I}$	$r(I,D) = 0.01$	$r(G,B) = 0.01$	1.28	0.6693	68	35

Table 4 – Characteristic points of the V-min diagram shown in Fig. 8.

Section	Split	Specified		Calculated			
		Recoveries		V_T/F	D/F	N	N_f
C1	$P_{E/I}$	$r(I,D) = 0.01$	$r(E,B) = 0.01$	0.51	0.4063	28	14
C2.1	$P_{E/H}$	$r(H,D) = 0.01$	$r(E,B) = 0.01$	0.56	0.3545	43	22
C2.2	$P_{G/I}$	$r(I,D) = 0.01$	$r(G,B) = 0.01$	0.65	0.4851	35	18
C3.1	$P_{E/F}$	$r(F,D) = 0.05$	$r(E,B) = 0.05$	1.06	0.3057	100	50
C3.2	$P_{G/H}$	$r(H,D) = 0.01$	$r(G,B) = 0.01$	0.76	0.4252	75	38
C3.3	$P_{H/I}$	$r(I,D) = 0.01$	$r(G,B) = 0.01$	1.13	0.6693	68	35

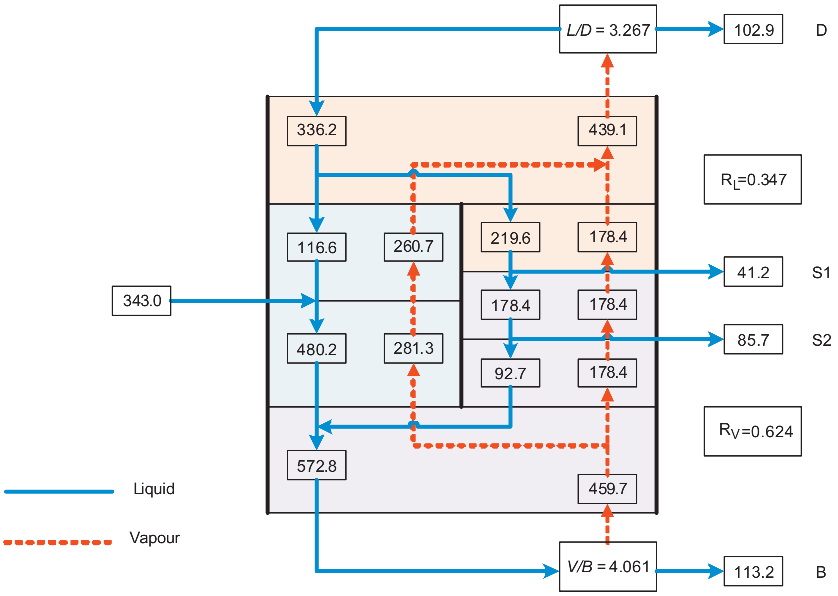


Fig. 6 – Mass balance for "2-4" configuration, with all internal vapour and liquid flows and splits according to V-min diagram.

tool that enables thorough and accurate assessment of potential for minimization of energy requirement of fully thermally coupled distillation columns. This rather simple method is based on assumptions of constant molar flows, infinite number of stages, and constant relative volatilities, and therefore holds for (near) ideal zeotropic mixtures. It relies on Underwood's equations utilised to estimate the value of theoretical minimum boil-up ratio, outgoing from the thermodynamic condition (*q*) and composition (*z*) of the feed and the *K*-values or equilibrium constants of each component for given operating conditions.

The real power of the V-min diagram is that it contains all necessary information to calculate the overall minimum energy requirement and all the internal flow rates for an optimally operated extended Petlyuk arrangement for an arbitrary multicomponent feed and any number of products (Halvorsen and Skogestad, 2003c). Here, Halvorsen and Skogestad have also shown that an optimally operated generalized Petlyuk arrangement results in the lowest overall vapour flow requirement for any distillation configuration when we consider constant pressure and no external heat integration.

We would generally anticipate that we would need to calculate the minimum energy for each succeeding column by a new column computation, but Halvorsen and Skogestad (2003b) showed that the properties determining minimum energy in each sub-column can be found from the previous column. This practically means that regardless the complexity of a situation, the V-min diagram containing all necessary information can be constructed based on feed data only. Importantly, this simple method that in original graphical form provides direct insight into the optimal separations behaviour in fully thermally coupled column arrangements can be easily translated into analytical form and implemented into a commercial process simulator, as it was done in present paper to generate reliable initial guesses for rigorous simulations.

The composition of the feed considered in this study is given in Table 2, with component *K*-values corresponding to feed stage conditions, and component grouping according to actual product specifications. For convenience, each component is represented by a letter according to alphabetic order. Distillate and bottoms stream are represented by common symbols *D* and *B*, while S_1 and S_2 denote molar flow rates of lighter and heavier side product, respectively.

The basic entity of the V-min diagram is a simple two-product distillation column at constant pressure with a given multicomponent feed (*F*), which at steady state implies two degrees of freedom in operation. There are several possibilities in this respect, however using the ratio of molar flow rates of internal vapour and the feed (*V*/*F*) and the ratio of molar flow rates of distillate product and the feed (*D*/*F*) appeared to be most appropriate choice. Namely, for each given pair (*D*/*F*, *V*/*F*) all other properties are completely determined, such as all component recoveries and product compositions.

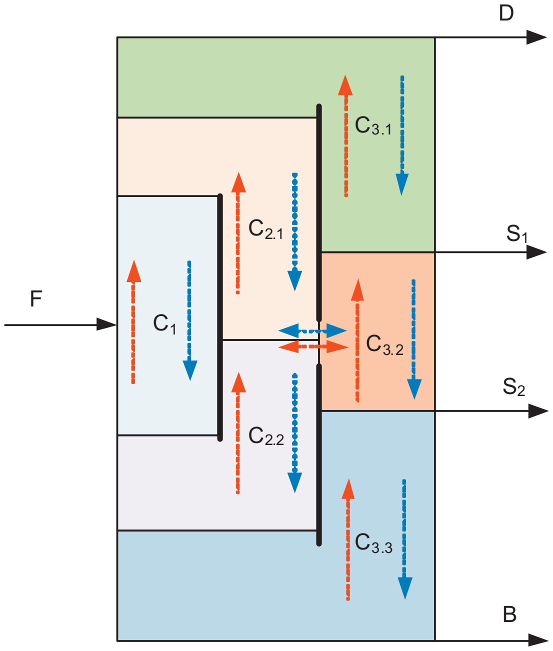


Fig. 7 – Partitioned part of a DWC according to "2-3-4" configuration, with three sections of main column superimposed on that representing "2-4" configuration.

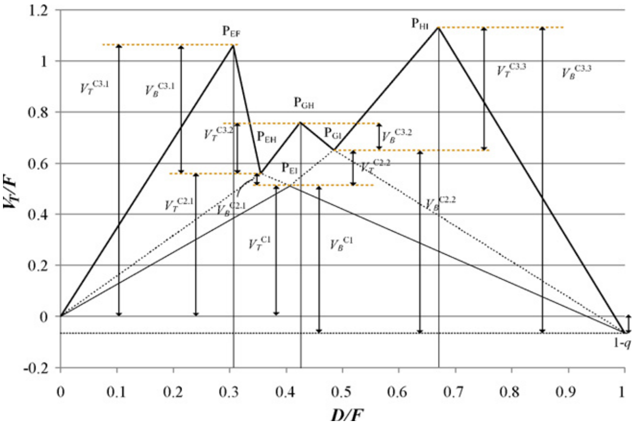


Fig. 8 – V-min diagram for “2-3-4” configuration.

3.2.1. V-min diagram for “2-4” configuration

The base case configuration shown in Fig. 1, consisting of a prefractionator and two final columns can be used to serve as basis to construct a V-min diagram. For convenience this situation is shown schematically in Fig. 4, with three independent columns represented as sections C_1, $C_{2.1}$ and $C_{2.2}$ i.e. the prefractionator, upper and lower column sections of a 4-p DWC shown in Fig. 2a. To ensure continuity, the upper and lower sections are connected via $N_{2,3}$ section, which is effectively operating at total reflux ($L = V$), without any net-transport of components, acting as a means for heat exchange between these two sections. The key components for the split (S_1/S_2) in the prefractionator are G/H, i.e. 3-methylhexane/toluene, and for splits (D/S_1) and (S_2/B) in respectively $C_{2.1}$ and $C_{2.2}$ are E/F (n-hexane/benzene), and H/I (toluene/ethyl benzene).

As is the case for a full Petlyuk arrangement (“2-3-4” arrangement), the overall vapour flow requirement for a “2-4” configuration is determined by the highest peak in the V-min diagram, shown in Fig. 5. For “2-4” configuration case, the required boilup however does not correspond to the one required for most difficult binary separation of the feed, because prefractionator is not operated at the preferred split, performing a sharp G/H split instead. This leads to increased energy requirements for E/F and H/I splits, which can be seen as higher V/F values compared to those of “2-3-4” configuration shown also in Fig. 5. The detailed analytical procedure is given by Halvorsen and Skogestad (2006).

If we subtract $(1-q)F$, which is negative (slightly sub-cooled liquid, i.e. $q = 1.0641$), from the value of highest peak in the diagram we will find that the required boilup is $V_{\text{min}}/F = 1.34$. Each sections vapour flow and net top product flow can be found directly as a difference between the peaks and knots in the V-min diagram. Note that the values of D and V are taken directly from the diagram, and other flows follow from simple mass balance expressions: $L = V - D$, $L_b = L + qF$, $V_b = V - (1-q)F$, $B = F - D$. Table 3 contains relevant specifications and outcomes.

A summary of the complete mass balance of “2-4” configuration is shown schematically in Fig. 6, indicating all internal vapour and liquid flows as obtained using V-min diagram. Given liquid and vapour splits represent fraction of respectively descending liquid and ascending vapour going to the prefractionator column side.

3.2.2. V-min diagram for “2-3-4” configuration

Internal layout of a DWC with “2-3-4” configuration is shown schematically in Fig. 7. Table 4 contains relevant data for characteristic points in V-min diagram shown in Fig. 8. First column shows the section, i.e. corresponding binary column, performing split indicated in second column, while the third column contains given specifications. The key components for the C_1 section, i.e. prefractionator column are n-hexane (E) as light, and ethylbenzene (I) as heavy key, respectively, and so on. As indicated in third and fourth column in Table 4, for all

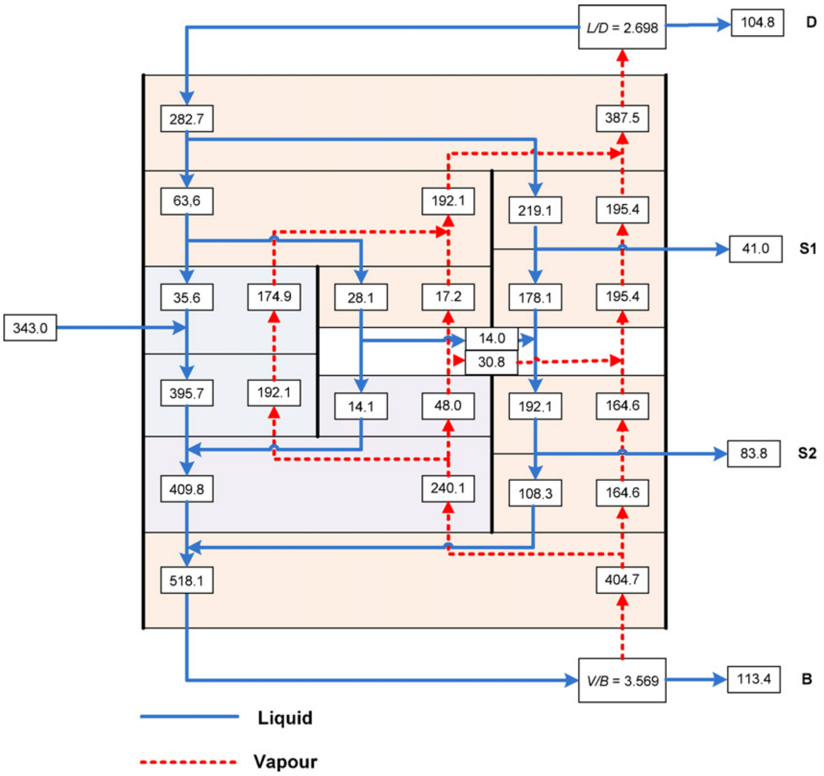


Fig. 9 – Mass balance of “2-3-4” configuration with all internal vapour and liquid flows according to V-min diagram.

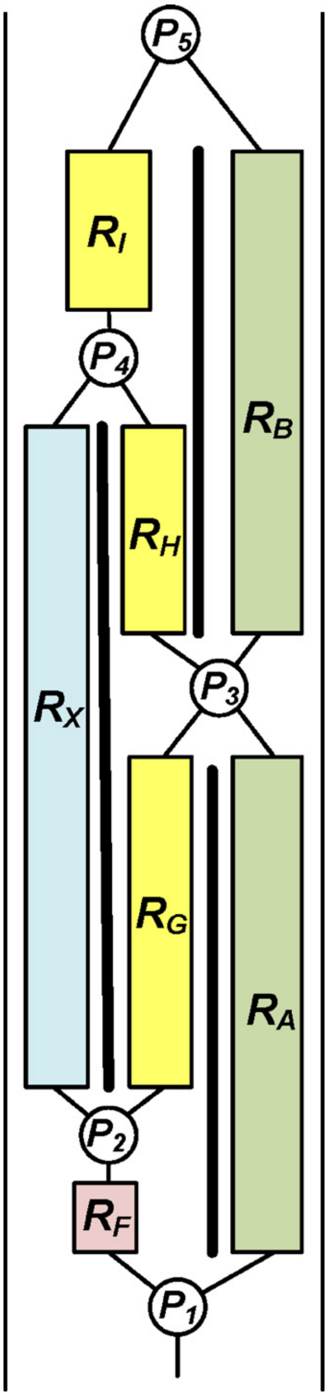


Fig. 10 – Schematic illustration of flow resistances in the partitioned part of a "2-3-4" DWC.

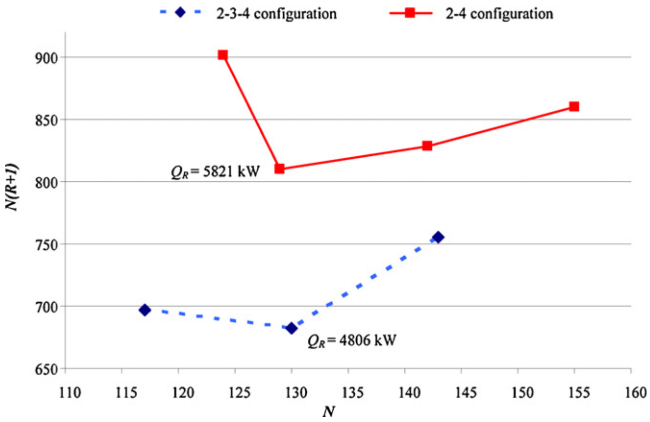


Fig. 11 – Optimum stage and reflux requirements for "2-4" and "2-3-4" configurations according to rigorous model calculations.

sections/columns except $C_{3,1}$, sharp splits have been chosen. Four columns on the right hand side of the Table 4 represent the results, i.e. characteristic vapour and top product flows associated with the numbers of stages employed in each of the columns.

The easy separation between the light key in the bottom product (*I*: ethylbenzene), and the heavy key in the top product (*E*: n-hexane) will determine the preferred split for the case, and thereby set the minimum vapour requirements for the prefractionator column. Practically speaking, by supplying the required vapour rate to an extended Petlyuk arrangement we get all the other products separated for "free", provided each sub-column in the structure is operated at its local "preferred split". That is, at minimum energy for separation of the light and heavy keys for that column while the intermediates distribute to both ends.

The split between toluene (*H*) and ethylbenzene (*I*), represented by the highest peak in V-min diagram shown in Fig. 8, requires the largest vapour flow rate, which means that this amount of vapour is generated by the reboiler and will be used for all separations involved. Internal mass balances are then used to determine each individual vapour and liquid load. For instance, the interaction between two sections of the central column and the middle section of the main column, i.e. $C_{2.1}$–$C_{3.2}$–$C_{2.2}$, is described by following balance expressions where the negative sign indicates stream going towards central column, and positive sign the stream going towards main column.

$$F_{V}^{C3.2} = V_{T}^{C2.2} - V_{B}^{C2.1} \tag{1}$$

$$F_{L}^{C3.2} = L_{B}^{C2.1} - L_{T}^{C2.2} \tag{2}$$

Subscripts V, L, B and T represent vapour, liquid, bottom and top of the column, respectively. Superscripts denote sections as shown in V-min diagram.

Fig. 9 shows schematically complete material balance of "2-3-4" configuration DWC, containing all internal flow rates of vapour and liquid streams obtained by V-min method. Corresponding vapour and liquid splits are not shown explicitly, because there are six on both liquid and vapour sides, and these can be calculated from data shown in Fig. 9. Note that this is much more complicated situation than in case of "2-4" configuration, with only one split of liquid and vapour streams.

The short-cut calculation procedure for initialization of rigorous simulation in "2-3-4" configuration case can be summarized as follows:

1. Choose key components and specify required recoveries.
2. Perform a series of rigorous binary distillation calculations to determine *D*/*F* and V_T/F values in points of interest in V-min diagram, for number of stages being at least $4N_{min}$.
3. Using simple mass balances, as indicated in Fig. 8, calculate required vapour and liquid flows.
4. The compositions of junction streams can be taken from appropriate product stream composition in binary distillation calculations or rather a few stages inside the binary column, just beyond the remixing zone arising from the presence of a condenser or reboiler.

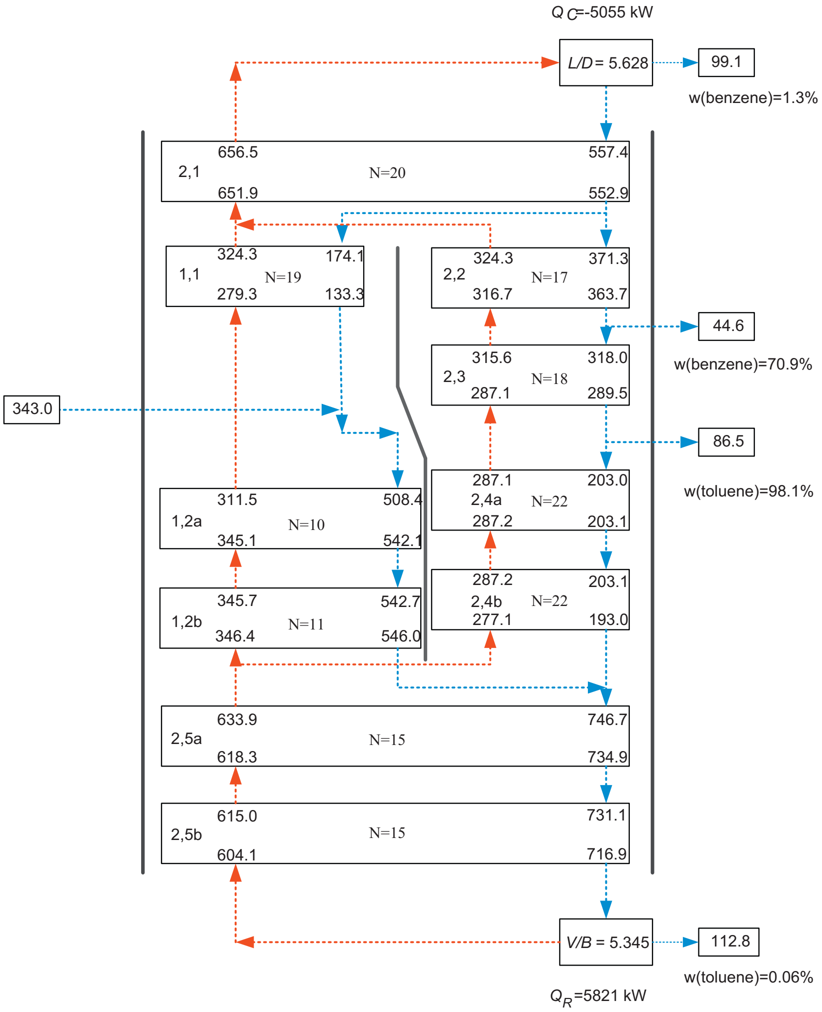


Fig. 12 – Mass balance of "2-4" configuration with all internal vapour and liquid flows according to rigorous model.

It should be noted that use of commercial process simulator for short-cut simulation of "2-4" configuration is not so straightforward. This case cannot be modelled as a series of binary distillation calculations of the same feed, because prefractionator column is not operated at a preferred split, causing higher energy use in subsequent sections. A way of performing simulations is to use the base case configuration in Fig. 1, but with liquid fractions of the feed into the final two columns set to the effective liquid fraction of the thermal coupling. This will give an artificial superheated feed to the upper column and an artificial sub-cooled feed to the lower column giving the same flow changes at the junctions as in the fully thermally coupled "2-4" configuration in Fig. 3. However, this may in some cases give convergence problems because the artificial temperatures may become close to critical values.

3.3. *Detailed modelling approach*

Sequences used for simulation of proposed configurations are shown in Fig. 3. All sections' stage numbers were initially set at effectively infinite values (>4$N_{\min}$). Side stream flows rates were initially set according to the material balance. Reflux ratio was adjusted to keep top and bottom products' purities at specified levels, and boil-up ratio was set to provide necessary vapour flow from the reboiler, as calculated from V-min diagram. Initial values of vapour and liquid split ratios were also set as calculated from V-min diagram, and then tuned in order to keep heavy key and light key recoveries in section's top and bottom respectively, below 0.01.

The actual number of stages was then found using following procedure. Keeping boil-up ratio constant, number of stages in each section was gradually reduced, to the values

Table 5 – Comparison of energy requirements of studied sequences, estimated using shortcut and detailed methods.

	Base case	"2-4"	"2-3-4"
Shortcut method			
$V_{\min}/F$	2.21	1.34	1.11
Relative savings in reboiler duty (%)	–	39.4	49.8
Rigorous method			
Total QR, [MW]	10.03	5.82	4.81
Total QR/F [MW/t]	0.324	0.183	0.152
Relative savings in reboiler duty (%)	–	42.0	52.0

Table 6 – Comparison of conventional and two DWC designs.

Configuration	Conventional			"2-4"	"2-3-4"
Column	C1	C2	C3		
Shell tangent to tangent height (m)	40.5	39.5	39.5	63.8	60.4
Shell diameter (m)	2.0	2.0	1.8	2.2	2.1
Top pressure (bar)	1.70	2.70	1.01	2.2	2.2
Pressure drop (bar)	0.313	0.272	0.244	0.150	0.137
Reboiler duty (MW)	3.76	3.12	3.15	5.82	4.81
Total reboiler duty (MW)	10.03	5.82	4.81		
Number of stages/trays	40/61	38/59	38/59	129/–	130/–
Number of packed beds	–	–	–	10 (7)	13 (10)
Number of distributors	–	–	–	10 (7)	11 (8)
Number of liquid catchers	–	–	–	8 (5)	9 (6)
Number of support grids	–	–	–	10 (7)	13 (10)

Note: Numbers in parentheses indicate devices placed in partitioned part of the column.

where product purities were still not compromised. Then, reboiler specification was changed to automatically adjust to keep bottom product purity. Number of stages in each section was proportionally reduced, and split ratios tuned to achieve desired side product purities.

Effectively, optimization has been performed by gradually minimizing (in each step) the product of the number of stages and the reflux ratio: $N(R+1)$, which represents a good approximation of total annualized costs.

Detailed calculation is effectively done following these steps:

1. Chose appropriate conventional column sequence.
2. Use values from V-min diagram, including stage number, for initialization.
3. Keeping product purities at specified levels, using split ratios to minimize reboiler duty.
4. Gradually reduce number of stages, repeating step 3, until $\min(N(R+1))$ is achieved.

3.4. *Dimensioning*

Dividing wall columns can be equipped with trays, random or structured packing, same as conventional columns, but peculiarities, i.e. essential details associated with hydraulics and consequently dimensioning of these columns are not described in open literature.

The basis for dimensioning is a converged column profile obtained by rigorous column steady-state simulation. This effectively means that liquid and vapour flows and properties are known for every column stage. In conventional column design, the dimensioning has to ensure stable column performance with regards to liquid and vapour loads. In DWCs, dimensioning has one additional purpose, and that is to ensure desired vapour split below the partition wall. Unlike liquid split, which can be set precisely by an external device, vapour split ratio is self-adjusting and is set by the governing pressure drops across different column sections. In other words, in order to be able to precisely tune the vapour split, the designer needs to be able to accurately predict and manipulate accordingly the pressure drop of column sections separated by the partition wall. In conjunction with the fixed liquid split, the pressure drop depends on the type and size of internals used. If a bed, sized to ensure given separation, does not generate sufficient pressure drop to ensure required vapour split, additional pressure drop can be arranged for instance by adjusting the free area of liquid distributors and/or catchers accordingly.

The "2-4" configuration appeared to be rather simple in this respect. Additional challenges are associated with present attempt to evaluate feasibility of a multiple-partition wall column, which means going beyond the limits of practical experience of J. Montz GmbH, the pioneer in this field among equipment manufacturers, which was involved with design and delivery of more than 90 packed DWCs so far.

Fig. 10 shows schematically flow resistances as encountered in the partitioned part of a "2-3-4" configuration DWC. In

Table 7 – Equipment and utilities cost, and total annualised cost (TAC) for "2-4" and "2-3-4" configurations.

Configuration Equipped with	Conventional Sieve trays	"2-4" Structured packings	"2-3-4" Structured packings
Total equipment costs ($)			
Shell	1,819,996	1,015,543	924,883
Internals	768,276	1,358,112	1,441,898
Reboiler	561,294	393,578	336,353
Condenser	637,547	264,245	272,759
Total	3,787,113	3,031,478	2,975,893
Savings	–	20.0%	21.4%
Operating costs ($/year)			
Cooling	577,257	108,103	86,632
Heating	986,355	752,127	620,980
Total	1,563,612	860,230	707,612
Savings	–	45.0%	54.7%
TAC ($/year)	1,942,323	1,163,378	1,005,201
Savings	–	40.1%	48.2%

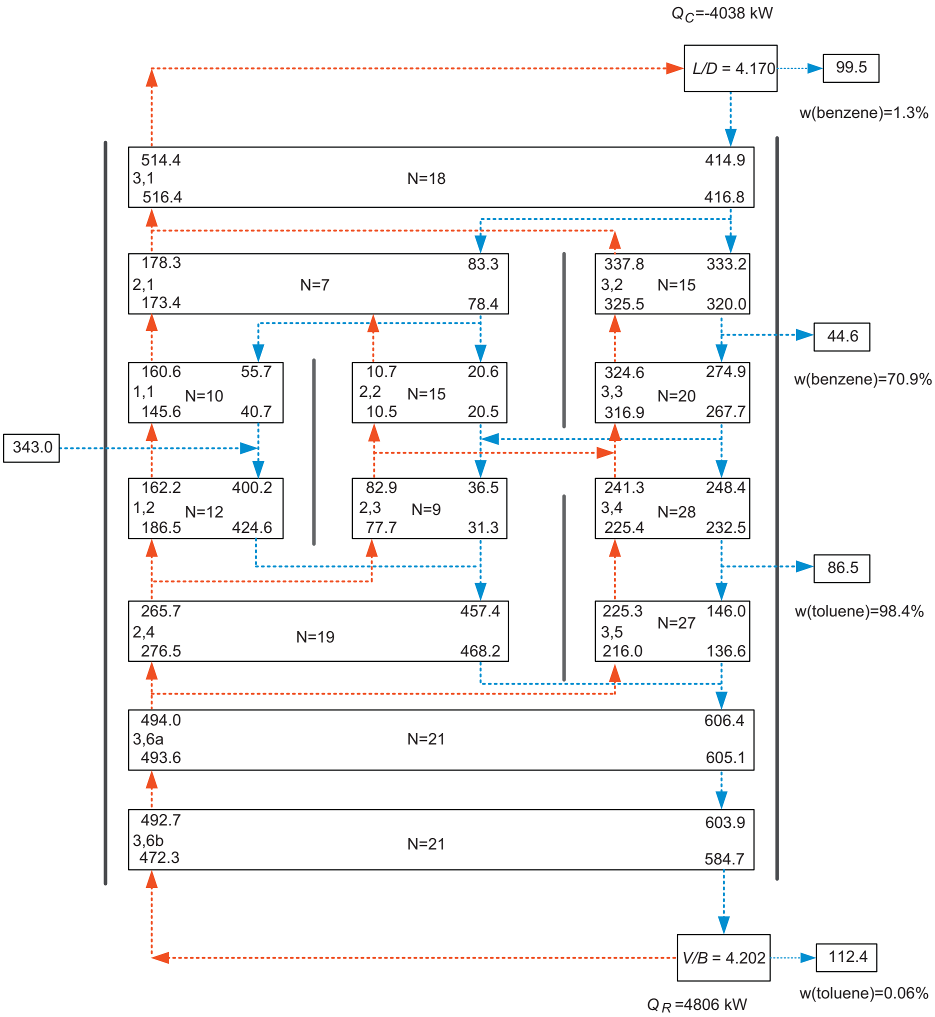


Fig. 13 – Mass balance of "2-3-4" configuration with all internal vapour and liquid flows according to rigorous model.

order to arrive at required vapour splits, following conditions must be satisfied:

$$\Delta p_{RF} + \Delta p_{RG} = \Delta p_{RA} \quad (3)$$

$$\Delta p_{RH} + \Delta p_{RI} = \Delta p_{RB} \quad (4)$$

$$\Delta p_{RX} = \Delta p_{RG} + \Delta p_{RH} \quad (5)$$

In present case, with pronounced differences in the number of stages and flow rates of phases in parallel sections of the column, different types and sizes of J. Montz corrugated metal sheet structured packings of series B1 have been considered to provide enough flexibility in this respect. Two basic structured packing area sizes were considered as appropriate for this case, 250 and 350 m^2/m^3, respectively, in conjunction with different corrugation inclination angles as well as designs, i.e. M and MN. For the same specific geometric area, using a packing with 60° instead of common 45° means a nearly factor three drop in the pressure drop, and a 30% higher capacity, at the expense of some 20% loss of efficiency (Olujić et al., 2002). Packings of series M have a long smooth bend at the end of the corrugations, which reduces the pressure drop and increases the capacity accordingly.

If this packing is used at vapour loads below the loading point then some 10% loss of efficiency should be accounted for with respect to standard version of the same specific geometric area. MN series combines a shorter smooth bend with a decreased corrugation inclination angle, generating additional pressure drop due to increased interaction of crossing vapour streams, which however translates into more efficiency, while preserving a rather high capacity. More detailed information on the performance characteristics of this new generation, high performance Montz structured packings can be found elsewhere, e.g. Olujić et al. (2010).

The dimensioning procedure for a packed DWC can be described as following:

1. Choose packing type.
2. Calculate required packing height in each section via HETP.
3. Find critical vapour load and use it to determine overall column diameter.
4. Adjust wall positions, until calculated pressure drop in all sections is below 3 mbar/m. If that is not achievable, increase overall column diameter.
5. Choose internals, using liquid loads for guidelines. Use chimney tray for side-stream draw-offs, regardless of liquid load.
6. Adjust free areas of collectors in divided section, to achieve equal calculated pressure drops, ensuring required vapour splits. If that is not achievable, adjust wall position, and repeat calculations.

3.5. Cost estimation

Similar to conventional columns, total DWC costs can be split into cost of shell, packings and auxiliary internals. The purchased cost of sieve trays, packings, liquid distributors, liquid catchers and packing support grids has been provided for the purpose of this and similar studies by J. Montz. The purchased cost of structured packings is based on the specific geometric area per unit volume, and for the present case, the base cost of standard packing with an area of 250 m^2/m^3, independent of the type, is US$ 2000/m^3. For larger geometric area packing considered in this study (350 m^2/m^3) this value needs to be multiplied by factor 1.4 corresponding to the ratio of two specific geometric areas. The base unit purchased cost for the liquid distributor is US$ 4000/m^2, for liquid catcher US$ 2000/m^2, and for packing support grid US$ 800/m^2.

Compared to conventional columns, the equipment related costs of a DWC are somewhat higher. For instance, the purchased cost of internals and packings placed in a DWC is higher because it includes partition walls and additional provisions needed to get packings and related internals ready for installation. For single-partition wall with sections placed off-centre the design complexity cost factor is 1.2 while for a multi-partition wall section of a DWC this value is higher, i.e. 1.3, with respect to conventional column. Purchased cost of equipment is multiplied by factor 2 to arrive at installed cost. These particular values are considered reasonable for present purposes.

Installed column shell costs for conventional tray columns and DWCs as well as reboilers and condensers have been determined using well established correlations from Douglas book (1988), expressed in SI units. The estimated installed costs have been updated using Marshall & Swift Index for 2009 (Chemical Engineering, 2010). The purchased cost for sieve trays as employed in design of three columns of the conventional configuration is US$ 600/m^2 and to obtain installed cost factor 3 is employed.

For the sake of simplicity, the operating costs are in present case taken to be that of the utilities, i.e. the heating medium and the cooling water. Since the bottoms temperature in present case is well above that of low and medium pressure steam, the same heating medium (furnace using fuel oil) is considered as in actual aromatics plant for conventional columns. The utilities prices adopted for this study are: US$ 130/tonne for fuel oil, and US$ 0.03/tonne for cooling water, and 13$/tonne for steam.

Total annualized cost (TAC) is based on 8322 operating hours per year and 10% of installed costs, assuming a plant (financial) life time of 10 years.

4. Results and discussion

The curves representing various stage and reflux requirement relations for main column side of configurations “2-4” and “2-3-4” are shown in Fig. 11, indicating respectively 129 and 130 equilibrium stages as optimum values. The reboiler duties corresponding to these points are also shown.

Energy requirements of conventional and two alternative DWC configurations are compared in Table 5. Interestingly, the rigorously estimated, reboiler duty based energy savings, expressed in percents, do not differ practically from those predicted by the short-cut method. Simpler design, i.e. “2-4” configuration ensures around 42% saving compared to conventional three-column configuration, while the saving achievable with complex design, i.e. ‘2-3-4” configuration, is around 52%. In other words, “2-3-4” configuration requires only one half of the energy to achieve the same separation as conventional configuration.

Compared to simpler “2-4” configuration, the thermodynamically optimal “2-3-4” configuration column requires 17.4% less energy for the same goal. This may be considered not attractive enough to move users to consider accepting the risks associated with building and operation of such a complex column. However, in present case this means an additional energy saving of 1 MW, and this number indicates a potentially higher financial benefit with respect to that expected from simpler single-partition wall configuration.

The optimized number of stages and corresponding inlet and outlet vapour and liquid mass flow rates for all beds in two configurations are summarized in Figs. 12 and 13, respectively. Compositions of product streams in all configurations satisfy requirements of the base-case situation, as indicated in Table 1. Namely, C5–C6 stream must contain less than 1.3 mass% benzene, and toluene stream more than 98.0 mass% toluene. Owing to the fact that approximate calculations have been performed with a relatively larger number of stages, both the reflux and boil-up ratios generated by detailed calculations (an optimised, i.e. minimised number of stages) are significantly higher. This implies larger internal liquid and vapour flows and these are, as expected, relatively larger for single partition wall configuration than for maximally energy efficient multiple-partition wall configuration. Consequently, the latter should require smaller column dimensions and consequently lower capital cost.

The liquid and vapour flow rates for the top and bottom of each bed, together with belonging physical properties, served as basis for column dimensioning. In both cases the bottom section with highest vapour and liquid loads was taken as basis for determination of the shell diameter. This in both cases appeared to be large enough to accommodate parallel sections, containing where necessary appropriate sizes and types of structured packing as well as liquid collecting devices, with free area chosen within given range to tune the pressure drop. Estimation of the pressure drop of various sizes and types of Montz packings used in conjunction with state of the art narrow trough liquid distributors and collectors was performed using methods that will be described in details in a forthcoming publication.

Detailed drawings of two columns are shown in Fig. 14, indicating relative size of packed beds in different sections as well as the type of liquid collector used. In general for specific liquid loads above 20 m^3/m^2 h a chimney type collector was used as well as for the draw-off of side products. Two beds in central section are rather narrow and practically rectangular, and with three beds in parallel above and below the side-draw-off a rather large fraction of walls is involved. Nevertheless, by combining in each layer conventional liquid scrappers with robust ones that also ensure fixing of the partition wall between two packed beds, bypassing of liquid and vapour, which is a serious concern, could be minimised.

Main column dimensions and the number of beds, distributors, collector and packing support grids contained in conventional and partitioned parts (numbers in parentheses) of “2-4” and “2-3-4” DWC are summarised in Table 6. For comparison, main dimensions of the three columns of the conventional configuration, designed as tray columns are also shown in Table 6.

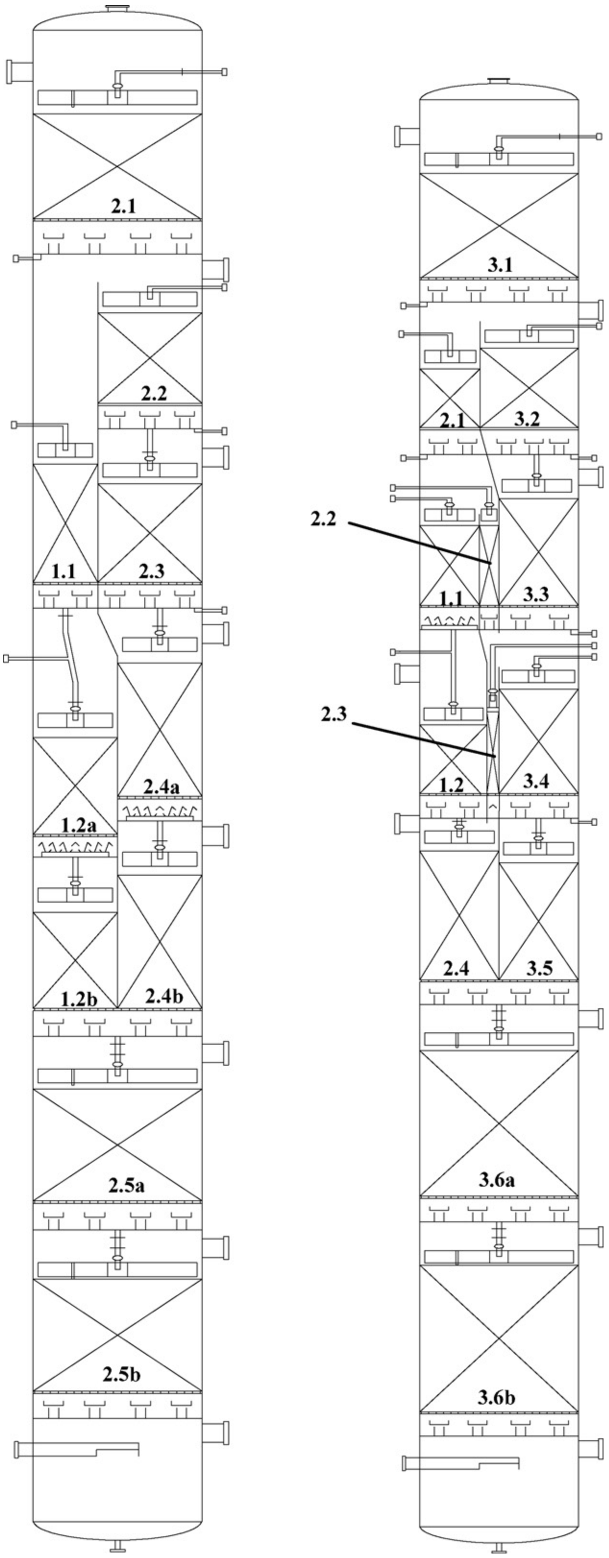


Fig. 14 – Detailed drawings of single (“2-4”) and multiple (“2-3-4”) partition wall DWCs. (numbers indicate individual beds as given in Figs 12 and 13, respectively).

The shells of two DWCs are taller but make roughly only one half of total height of three columns from conventional sequence. Diameters of both DWCs are slightly larger, and the reduced energy requirement of complex “2-3-4” configuration, i.e. reduced internal vapour flow rate, results in a somewhat smaller diameter. Due to a more compact arrangement of the partitioned part, the complex DWC is also shorter than the single partition wall “2-4” configuration column.

As shown in Table 7, compared to conventional, three columns configuration, capital cost of two compact dividing wall columns is approximately 20% lower, which is a less pronounced saving than usually experienced with conventional three-product DWCs. This however is mainly due to cost enhancement factors adopted to account for additional manufacturing and construction/installation complexity associated with single and multi-partition, off-centre wall DWCs configurations. Owing to a rather pronounced operating cost reduction, i.e. 45.0% and 54.7% for respectively “2-4” and 2-3-4” configuration, the corresponding savings expressed on TAC basis are quite large, i.e. 40.1% and 48.1%.

Regarding the fact that the operating (energy) cost of the “2-3-4” configuration is 17.7% lower, compared to that of the “2-4” configuration, which results in a 13.6% lower TAC, it appears that complex, multi-partition wall configuration is an attractive option for present case.

Regarding the control aspects of four product columns, which however is not within the scope of the present paper, one should note that so far only one DWC with “2-4” configuration has been realized in industrial practice (Kaibel et al., 2007; Olujić et al., 2009; Dejanović et al., 2010a). For such a column Strandberg et al. (2010) have shown a feasible control strategy based on controlling four temperatures by manipulating the liquid split and the three upper product flow rates while boilup and vapour split are kept constant. It is reasonable to extend this strategy to the full “2-3-4” column. This however is subject of an ongoing research effort at NTNU under supervision of two of the co-authors of the present paper, which will be addressed soon in extension of their previous work along this line.

5. Conclusions

An energy efficient alternative has been proposed for recovery of essential fractions in a refinery aromatics complex. Three columns configuration has been replaced by one DWC for obtaining four products. Two options, one with a single longitudinal partition wall, with some sections off-centre, and a multiple-partition wall column containing three sections in parallel have been worked out using rigorous simulations initiated using the values of governing variables estimated using an established short-cut method.

V-min diagram proved to be a simple and effective tool for identification and conceptual design of internal, minimum energy requirement configuration of a multi-product DWC, as well as for reliable initialization of detailed (rigorous) calculations.

Detailed calculation method adopted, in conjunction with a simple empirical objective function for design optimality indication, allows easy determination of the stage and reflux requirement of a complex DWC. The dimensioning method developed for standard, three-product columns appeared to be an effective tool for design and assessment of cost-effectiveness of alternative internal configurations of four-product multiple partition wall DWC equipped with structured packings.

The simulation studies indicated a strikingly large energy saving potential compared to conventional configuration, resulting in a 40.1% and 48.2% lower TAC for single- and multiple partition wall DWC, respectively. This means that more complex, multiple-partition wall column is a more attractive option for industrial implementation, but due to its constructional complexity it may appear impractical.

Regarding the scale of this and similar applications, additional 17.7% saving in operating costs translates into large financial benefits. Therefore in present and similar cases there may be a strong incentive to put more effort and resources into overcoming potential barriers and making multiple-partition wall DWC configurations industrially viable.

Thanks to the availability of proven non-welded, self-fixing partition wall structured packing technology, multiple partition wall configurations could be realized in practice. If it appears that control of the complex DWCs (subject of an ongoing research effort at NTNU) will not be too demanding (impractical), than the barriers other than technical need to be overcome to enable practical implementation of this highly sustainable distillation column technology.

Acknowledgement

The authors would like to thank INA Refinery Sisak, Croatia, member of MOL Group for providing actual plant data for the purposes of this study.

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