# CONCEPTUAL DESIGN AND COMPARISON OF FOUR-PRODUCTS 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 aromatic's mixture can be separated very efficiently into four fractions according to 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 (actual delivery prices) cost estimation. Comparison of total annualized costs indicates that more energy efficient complex configuration with three partition walls is a viable option in present case.

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<sup>1</sup>. 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<sup>2</sup>. 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 additional entropy of mixing formation due to internal re-mixing of streams. Its special feature is that it is the only known process 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<sup>2,3</sup>. 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 distribution of vapour among parallel sections along the column shell can be controlled only by adjusting the pressure drop of each partitioned section accordingly, which is however difficult to achieve in practice.

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<sup>4</sup> 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.

#### 1.1 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 product. The separation 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, with feed reduced to 15 representative components<sup>5</sup>. In order to acquire a base-case design for a four-product sequence, a third column was added, in which separation of heavy platformate into toluene and ethylbenzene and heavier components takes place. Thus the separation is performed according to the arrangement shown in Fig. 1a, which is regarding energy consumption similar to equivalent direct sequence. It can be easily implemented, simply by adding the 3<sup>rd</sup> column, without changing the operation of the existing sequence. Product stream compositions obtained by simulation of this three-column configuration are presented in Table 1.

Stream Name	Feed	C5-C6	BRC	Toluene	Heavy
Temperature, [°C]	100.01	40.00	119.10	111.29	163.32
Pressure, [bar]	2.90	5.70	3.17	1.01	1.56
Total flow					
[kmol/h]	343.0	97.8	47.1	86.5	111.6
[kg/h]	31730.0	7443.4	3874.9	8001.0	12409.2
Component mass fractions					
N-Hexane and lighter	0.2517	0.9869	0.1642		
Benzene	0.0855	0.0131	0.6750	-	-
3-Methylhexane	0.0204	-	0.1608	0.0026	-
Toluene	0.2474	-	-	0.9718	0.0061
Ethylbenzene and heavier	0.3950			0.0256	0.9939

Table 1. Base case stream table

## 2. Possible DWC configurations

Base case sequence and investigated options are shown in Figure 1. Figure 1b shows a so-called Kaibel or a "2-4" configuration, and Figure 1c fully-extended, four-product DWC, or a "2-3-4" configuration. The former enables a significant energy saving with respect to conventional configuration, which however is well below the saving achievable with a fully-extended counterpart. However its simpler design, construction and operation make it an interesting alternative. Such a DWC is in operation for more than two years in a BASF plant<sup>2</sup>. The complexity of "2-3-4 configuration" is the main reason that there are no known applications in industrial practice to this day. An impression on internal configurations of single- and multiple-partition wall configurations is given in Figs 1b and 1c, respectively.

In addition these figures indicate the number of governing variables associated with these two configurations. The initial estimates of these variables are required to facilitate rigorous calculations, using commercial software by employing corresponding thermodynamically-equivalent sequences of simple columns, shown in Figs 2a and 2b, respectively. So called "2-4 configuration" requires 13, whereas "2-3-4 configuration" requires a total of 22 parameters. In order to get feasible values, a robust design-oriented short-cut method is required, like the so-called V<sub>min</sub> diagram method introduced recently by Halvorsen and Skogestad<sup>6-8</sup>. This method is based on assumptions of constant molar flows, infinite number of stages, and constant relative volatilities and utilises Underwood's equations to estimate the value of theoretical minimal boil-up ratio, outgoing from the composition of the feed and corresponding equilibrium constants of each component. Application of this method to present case is described and discussed in detail in another paper<sup>4</sup>. A practical benefit of this method that it can be

easily implemented into a commercial process simulator, as it was done in present paper to generate reliable initial guesses for rigorous simulations.



Figure 1. Base case sequence and investigated DWC configurations

### 2.1 Rigorous simulation

Sequences used for simulation of proposed configurations are shown in Figure 2. All sections stage numbers were initially set at effectively infinite values (4\*N<sub>min</sub>). Side stream flows were 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. First, column concentration profiles of key components were inspected to estimate number of stages in each section that do not contribute significantly to separation. Keeping boil-up ratio constant, number of stages in each section was gradually reduced, to the values 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.



a) 2-4 b) 2-3-4 Figure 2. Simple column sequences used for rigorous simulation

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.

#### 2.2 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 insure stable column performance with regards to liquid and vapour loads. In DWCs, dimensioning has one additional purpose, and that is to insure desired vapour split across the 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 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 additional challenges in this respect, associated with present attempt to evaluate feasibility of a multiple-partition wall column push also behind 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 80 packed DWCs so far.

In present case, with pronounced differences in the number of stages and flow rates of phases in different sections of the columns, different types and sizes of J. Montz corrugated metal sheet structured packings of series B1 have been utilised. Two basic structured packing sizes were used,  $250 \text{ and } 350 \text{ m}^2/\text{m}^3$ , respectively, in conjunction with different corrugation designs, i.e. M and MN. For the same specific geometric area, the former generates less pressure drop at the same vapour and liquid load, while the latter one translates additional pressure drop into more efficiency, while preserving a rather high capacity. More detailed information on the performance characteristics of these new generation, high performance Montz structured packings can be found elsewhere in this book<sup>9</sup>.

#### 2.3 Cost estimation

Similar to conventional columns, total DWC costs can be split into cost of shell, packings and auxiliary internals. The purchased cost of the column shell, packings, liquid distributors, liquid catchers and packing support grids has been determined using J.Montz in-house preliminary cost estimating method, which is within 5 per cent accuracy with respect to final delivery price. Compared to conventional columns, the costs of a DWC are somewhat higher. For instance, the purchase cost of a shell for a DWC shell is approximately 20 per cent higher than that of conventional counterpart. The same is with internals which need to be adapted to geometry as imposed by placing partition walls, which are in four products column mainly or fully placed in off-centre positions. In general distributors, catchers and grids placed in the partitioned part of a DWC cost 30 per cent more than conventional counterparts. The latter can, in a DWC, usually be found in columns sections above and bellow the partition wall. The purchase 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<sup>3</sup>. For larger geometric area packing considered in this study this value needs to be multiplied by factor 1.4 (ratio of two specific geometric areas). The base unit purchase cost for the liquid distributor is US\$ 4000/m<sup>2</sup>, for liquid catcher US\$ 2000/m<sup>2</sup>, and for packing support arid US\$ 800/m<sup>2</sup>.

Purchased costs of the reboiler and condenser have been estimated using correlations available in Chemcad. 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 cooing 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. Therefore the prices provided by INA refinery have been used as basis for evaluation of total annualized costs (TAC) associated with two feasible configurations of DWC. These are US\$ 362/tonne for fuel oil, and US\$ 0.33/tonne for

cooling water. 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.

#### 3. Results

Comparison of thermal performance of studied configurations and the base case is shown in Table 2. Striking is the amount of energy saving associated with more practical 2-4 DWC configuration, which however can be further enhanced significantly (17.4 %!) by implementing more complex 2-3-4 configuration.

Table 2. Comparison of studied sequences					
	Base case	"2-4"	"2-3-4"		
Total Qr, [kW]	9520	5821	4807		
Total Qr/F [kW/t]	0.301	0.164	0.151		
Relative savings in reboiler duty	-	38.9%	49.5%		

Regarding the fact that in present industrial case additional 1 MW energy can be saved there is a strong incentive to consider implementing more complex, multiple-partition wall configuration. Interestingly, the rigorously estimated energy savings expressed in percents differ slightly from those predicted by the short-cut method<sup>4</sup>. The number of stages and inlet and outlet vapour and liquid mass flow rates of all beds in two configurations are summarized in Fig. 3.



Figure 3. Internal configuration with stage numbers for each section and corresponding vapour and liquid flow patterns for single- and multiple-partition wall DWC, including mass flow rates (kg/h) of the feed and four product streams

Configuration	"2-4"	"2-3-4"
Shell diameter (m)	2.2	2.1
Shell height (m)	63.4	66.4
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)

**Table 3.** Dimensions and components of two DWC configurations

Note: Numbers in parentheses indicate devices placed in partitioned part of the column. The overall dimensions of two shells are similar, and the reduced energy requirement of the complex configuration is visible through reduced internal vapour flow rates in a somewhat smaller diameter. This compensates in costs for somewhat taller column, and from Table 4 it can be seen that investment costs for two columns are similar. A lower utility cost is reflected in a correspondingly lower TAC (15.8 %!), which means that complex configuration is an attractive option for present case.

Configuration		"2-4"	"2-3-4"				
	Units						
Installed equipment costs							
Column shell	\$	2 934 400	2 908 200				
Column internals	\$	2 638 235	2 589 381				
Reboiler	\$	1 150 796	977 416				
Condenser	\$	186 042	70 805				
Total	\$	6 909 473	6 545 802				
Operating costs							
Cooling water	\$/year	1 189 130	952 128				
Fuel oil	\$/year	1 940 091	1 605 696				
Total	\$/year	3 129 221	2 557 824				
TAC	\$/vear	3 820 168	3 212 404				

**Table 4.** Equipment and utilities cost, and total annualised cost (TAC) for

 2-4 and 2-3-4 configurations (price reference January 2010)

# 4. 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. The simulations indicated a strikingly large energy saving potential compared to conventional configuration. In this respect, more complex, multiple-partition wall column is more attractive, because it maximizes the potential gain. Most importantly, thanks to the availability of proven non-welded, self-fixing partition wall structured packing technology, this complex configuration, which ensures shorter pay-back time than more practical single-partition wall configuration, can be realized in practice as a packed column.

## References

- 1. J. L. Humphrey and G. E. Keller II, *Separation Process Technology*, McGraw-Hill, New York, 1997.
- 2. Ž. Olujić, J. M. Jödecke, A. Shilkin, G. Schuch and B. Kaibel, *Chem. Eng. Process.* 48 (2009)1089-1104.
- 3. I. Dejanović, Lj. Matijašević, Ž. Olujić, *Chemical Engineering and Processing* (2010), doi:10.1016/j.cep.2010.04.001.
- 4. I. J. Halvorsen, I. Dejanović, Lj. Matijašević, Ž. Olujić, S. Skogestad, Distillation & Absorption 2010 (Editors: A. de Haan, H. Koijmaan, A. Gorak)
- 5. I. Dejanović, Lj. Matijašević, Ž. Olujić, ESCAPE-20 (Editors: S. Pierucci and G. Buzzi Ferraris), 2010 Elsevier, in print.
- 6. I. J. Halvorsen and S. Skogestad, *Ind. Eng. Chem. Res.* 42 (2003) 596-604.
- 7. I. J. Halvorsen and S. Skogestad, *Ind. Eng. Chem. Res.* 42 (2003) 605-615.
- 8. I. J. Halvorsen and S. Skogestad, Ind. Eng. Chem. Res. 42 (2003) 616-629.
- 9. Ž. Olujić, T. Rietfort, H. Jansen, B. Kaibel, E. Zich, G. Ruffert, T. Zielke, Distillation & Absorption 2010 (Editors: A. de Haan, H. Kooijman, A. Gorak).