Modelling of a dividing-wall distillation column and comparisonwith conventional 2-columns distillation system using EMSO software

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Conventional distillation columns models are composed of a large number of nonlinear differential-algebraic equations.Divided wall column (DWC) design presents an additional challenge for their modeling and optimization because much more equations are needed. However, the DWC can save up to 40% of the reboiler energy consumption [1]. Despite this advantage, DWC models are not readily available in commercial software, such as Aspen Plus© and HYSYS Process©. Hence, the usual representation of DWC in analysis and simulation reports in the literature is made with coupling of conventional distillation column models.

The aim of this work was to create a DWC model (Figure 1b) in an equation-oriented process simulator, free of charge to academic research and educational activities. This software, EMSO, has also the advantage that all developed models are open for inspection and extension by any user, which makes it extremely flexible for research use [2, 3]. A sensitivity analysis of streams composition and heat duties is then performed concerning design (total number of trays and number of divided trays) and operating (reflux ratio) parameters. Results are also compared to those obtained by a model of conventional 2-columns distillation system (Figure 1a) in the same software.

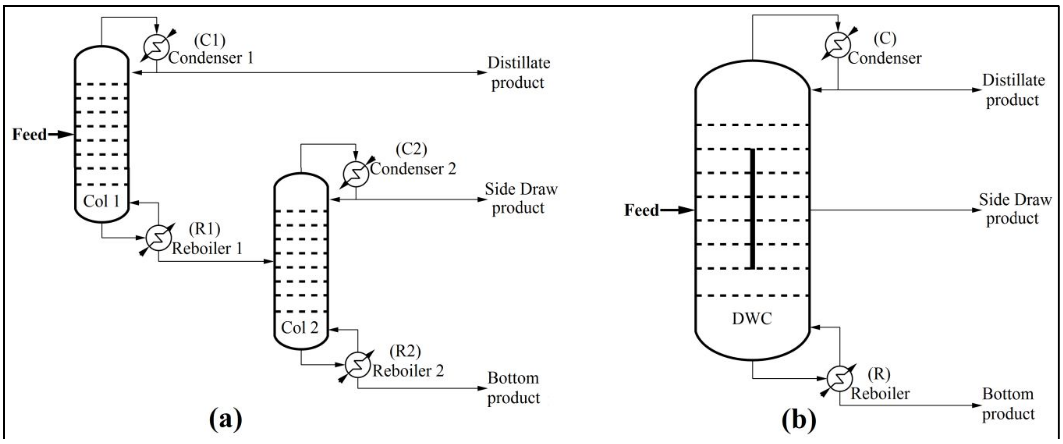

Figure 1.Application of distillation schemes(a) Conventional 2-columns and (b) DWC.

The models wereused to separate 480 kmol/h of a ternary equimolar mixture (n-pentane, n-hexane, n-heptane)using the Peng-Robinson state equation to predict the thermodynamic properties,and the boiling point of the mixture to calculate the temperature of each tray.In both schemes, each output stream has a flowrate of 160.00 kmol/h and the columns are operating at 510 kPa. Steady state results were obtained using the dynamic models with 8.3 h of simulation to generate good initial guess for the Newton method to obtain the steady state.

In the conventional 2-columns scheme, Column 1 (Col 1) has 20 trays with the feed in the 9th tray.Its bottom product feeds the 7thtray of Column 2 (Col 2), which has16 trays. A reflux ratio (RR) of 3.00 is used in both columns.

According to Table 2, the DWC was defined with 27, 47 or 107 trays. The RR as well as the number of divided trays were evaluated to maintain the same separation (molar fractions in the outlet streams) performed by the conventional 2-columns scheme (Table 1). The downward liquid flow is equally divided at the inlet ofthe divided trays, and the same happens to the upwardvapor.The inlet stream and outlet side draw product are positioned in the central tray of the DWC, in opposite sides of the dividing wall.

Table1–Molar fractions products and heat duties for the conventional distillation scheme.

		Distillate product	Side draw product[1]	Bottom Product[2]	Total condenser duty (kW)	Total reboiler duty (kW)
Conventional system	n-C5	0.983	0.036	0.000	8419.24	9510.11
	n-C6	0.017	0.897	0.077		
	n-C7	0.000	0.067	0.923		

[1]Distillate and [2]Bottom product of Col 2 in the conventional 2-column scheme.

Table 2 – Molar fractions products and heat duties for the DWC distillation scheme.

	Total number of trays	Divided trays	Reflux Ratio		Distillate Product	Side draw product	Bottom Product	Total condenser duty (kW)	Total reboiler duty (kW)
DWC	27	10	7.40	n-C5	0.983	0.037	0.000	8324.94	10034.8
				n-C6	0.017	0.898	0.075		
				n-C7	0.000	0.065	0.925		
	47	31	6.11	n-C5	0.983	0.037	0.000	7044.27	8495.86
				n-C6	0.017	0.896	0.077		
				n-C7	0.000	0.067	0.923		
	107	91	6.10	n-C5	0.983	0.037	0.000	7035.92	8482.29
				n-C6	0.017	0.898	0.075		
				n-C7	0.000	0.065	0.925		

The results show that DWC is able to obtain separation equivalent to those of the conventional 2-columns distillation system, even with smaller number of trays. Though the capital investment is lower due to the smaller number of trays, with few trays it is necessary a much larger RR, increasing the operating cost.With RR approximately twice that of the conventional 2-columns system, it is possible to obtain the same separation with 10.66% less of total reboiler duty by a column 30.5% higher, if the comparison is made to the sum of the number of trays of the two conventional.

In this way, a proper DWC model, easily editable by any user,was developed and is available inanopen-source software.

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References:

[1] Sangal, V. K.; Kumar, V.;Mishira, I. M. Optimization of a dived wall column for the separation of C4-C6 normal paraffin mixture using box-behnken design.*Chem. Ind. & Chem. Eng. Q. (Online)*, v. 19, n. 1, p. 107-119, 2013.

[2] Soares, R. P.; Secchi, A.R. EMSO: A new environment for modelling, simulation and optimisation. *Comp. Aid. Che.Engng*.p. 947-952, 2003.

[3] Rodrigues, R.; Soares, R.P.; Secchi, A.R. Teaching chemical reaction engineering using EMSO simulator. *Comput.Appl. Eng. Educ.* v. 18, n. 4, p. 607–618, 2010.