Influence of the main operating parameters on the DRPSA process design based on the Equilibrium Theory

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Supplementary material

The detail of the boundary conditions for each step are reported in Table S1, referring to the mathematical model and the numerical approach discussed in the paper.

Table S1: BCs for each step.

Step	BCs
BD	$z = 0 \rightarrow \bar{u}_{\frac{1}{2}} = 0$ $y_{\frac{1}{2}} = y_1$
	$z = 1 \rightarrow \bar{P}_{N+\frac{1}{2}} = P(t)/P_{rif}$
PU	$z = 0 \rightarrow \bar{u}_{\frac{1}{2}} = u_{LR}/u_{rif}$ $y_{\frac{1}{2}} = y_{i,L}$
	$z = 1 \rightarrow \bar{P}_{N+\frac{1}{2}} = P_L/P_{rif}$
PR	$z = 0 \rightarrow \bar{P}_{\frac{1}{2}} = P(t)/P_{rif}$ $y_{\frac{1}{2}} = y_{i,H}$
	$z = 1 \rightarrow \bar{u}_{N+\frac{1}{2}} = 0$
FE	$z = 0 \rightarrow \bar{u}_{\frac{1}{2}} = u_{HR}/u_{rif}$ $y_{\frac{1}{2}} = y_{i,H}$
	$z = 1 \rightarrow \bar{P}_{N+\frac{1}{2}} = P_H/P_{rif}$
Lateral feed injection	$z = z_{feed}^{-} \rightarrow \bar{P}_{n_{feed}+\frac{1}{2}} = \bar{P}_{(n_{feed}+1)-\frac{1}{2}}$
	$z = z_{feed}^{+} \rightarrow y_{i.(n_{feed}+1)-\frac{1}{2}} = \frac{y_{i,feed} \cdot \bar{u}_{feed} \cdot \bar{P}_{feed} + y_{i,n_{feed}+\frac{1}{2}} \bar{u}_{n_{feed}+\frac{1}{2}} \cdot \bar{P}_{n_{feed}+\frac{1}{2}}}{\bar{u}_{(n_{feed}+1)-\frac{1}{2}} \cdot \bar{P}_{(n_{feed}+1)-\frac{1}{2}}}$ $\bar{u}_{(n_{feed}+1)-\frac{1}{2}} = \frac{\bar{u}_{feed} \cdot \bar{P}_{feed} + \bar{u}_{n_{feed}+\frac{1}{2}} \cdot \bar{P}_{n_{feed}+\frac{1}{2}}}{\bar{P}_{(n_{feed}+1)-\frac{1}{2}}}$

The initial conditions requires arbitrary axial profiles of each state variable, while the molar fractions $y_{i,L}$ and $y_{i,H}$ are computed in accordance with the material balances in the two tanks, ϑ_1 and ϑ_2, as discussed in detail in (Rossi et al., 2019a).

In Table S2, the simulation results in terms of purity of A and B are reported for all the simulated separation processes, with $y_{A,feed} = 0.79$. The operating conditions are graphically reported in the $z_{feed} - C$ plane in the paper (Figure 3). Note that, being the heavy product flowrate constant and equal to the heavy molar flowrate in the feed, the purities of the two species are always equal to their recoveries.

Table S2: Purity obtained for each simulation reported in Figure 4 and 5 in the paper.

z_{feed}	C	Purity of A (equal to the Recovery of *A*)	Purity of B (equal to the Recovery of *B*)
0.069	0.09	0.983	0.924
0.069	0.12	0.903	0.625
0.069	0.15	0.862	0.476
0.069	00.18	0.844	0.409
0.094	0.12	0.987	0.936
0.094	0.15	0.92	0.69
0.094	0.18	0.878	0.534
0.138	0.12	1	1
0.138	0.15	0.996	0.972
0.138	00.18	0.984	0.927
0.138	00.21	0.934	0.742
0.138	0.24	0.897	0.604
0.194	0.09	0.995	0.968
0.194	0.12	0.986	0.935
0.194	0.15	0.978	0.903
0.194	0.18	0.971	0.878
0.194	0.21	0.966	0.859
0.194	0.24	0.962	0.844
0.25	0.03	0.990	0.974

0.25	0.06	0.981	0.914
0.25	0.09	0.97	0.875
0.25	0.12	0.963	0.847
0.25	0.15	0.957	0.827
0.25	0.18	0.953	0.813
0.25	0.21	0.95	0.801
0.25	0.24	0.948	0.793
0.306	0.03	0.951	0.804
0.306	0.06	0.945	0.783
0.306	0.09	0.942	0.770
0.306	0.12	0.939	0.762
0.306	0.15	0.938	0.756
0.306	0.18	0.937	0.751
0.306	0.21	0.936	0.748
0.306	0.24	0.935	0.745
0.362	0.03	0.913	0.662
0.362	0.06	0.915	0.670
0.362	0.09	0.918	0.683
0.362	0.12	0.92	0.690
0.362	0.15	0.922	0.695
0.362	0.18	0.922	0.699
0.362	0.21	0.923	0.701
0.362	0.24	0.924	0.703
0.418	0.03	0.912	0.661
0.418	0.06	0.912	0.66
0.418	0.09	0.911	0.657
0.418	0.12	0.91	0.654
0.418	0.15	0.91	0.653
0.418	0.18	0.911	0.658
0.418	0.21	0.913	0.664
0.418	0.24	0.915	0.670

0.474	0.03	0.912	0.661
0.474	0.06	0.912	0.66
0.474	0.09	0.911	0.657
0.474	0.12	0.910	0.654
0.474	0.15	0.910	0.652
0.474	0.18	0.910	0.65
0.474	0.21	0.909	0.648
0.474	0.24	0.908	0.646

Interpolation details

For the isopurity lines definition, a two-dimensional interpolation should be carried out. In fact, the steady state composition varies with C, at constant z_F, and vice versa. The problem has been faced combining both interpolation and data fitting, as shown for an illustrative example in Figure 5. In this case, the curve at constant purity equal to 0.85 is desired. Therefore, at $C = 0.18$, a linear interpolation between 0.878 and 0.813 is performed. The same is done at fixed $C = 0.21$ and then $C = 0.24$. Once that the z_{feed} values corresponding to a purity 0.85 is derived for each C value, ($*$ points in the figure), the data are fitted so that to obtain the constant purity curve (-- in the figure).

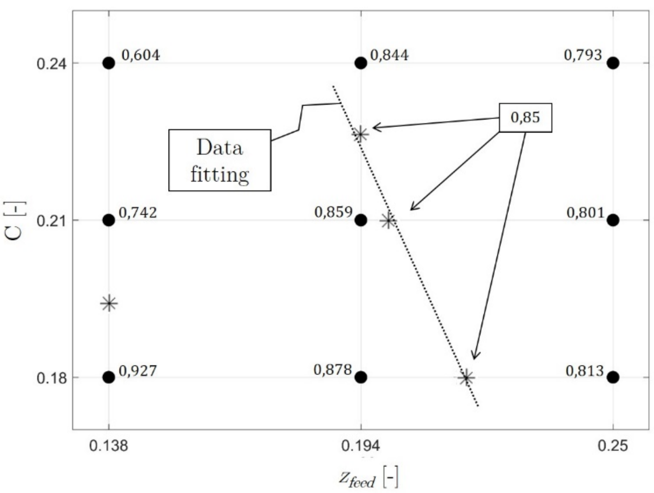

Figure S1: Interpolation example. (*) interpolated data, (o) simulated points

Different feed mixtures results

In Figure S2, the TOZs corresponding to the 96% purity of the heavy component are reported.

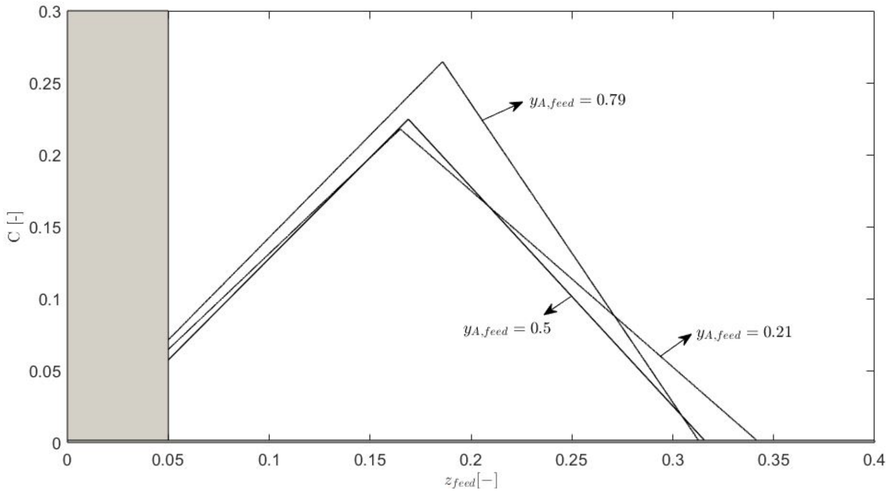

Figure S2: Heavy product constant purity= 96%, for the different $y_{A,feed}$ investigated