Electronic Supplementary Material

Separation of *n*-heptane/isobutanol via eco-efficient vapor recompression-assisted distillation: process optimization and control strategy

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Table S1 onomical evaluation of necessary parameters and formulas[1-3]

Items	Formulas and values
Tower diameter/m	Calculated by Tray Sizing in Aspen Plus
Length/m	$0.61 \times (N_T - 2) \times 1.2$
Column vessel cost/$	$\frac{M\&S}{280} \times 937.636 \times D^{1.066} \times H^{0.802} \times (2.18 + F_c)$
	$F_c = F_m F_p$, F_m=3.67; F_p = 1
Plate cost/$	$\frac{M\&S}{280} \times 97.243 \times D^{1.55} \times H \times F_c$
	$F_c=F_s+F_t+F_m$; F_s=1.0; F_t=0(sieve plate column); F_m=1.7
Heat exchanger cost/$	$\frac{M\&S}{280} \times 474.668 \times A^{0.65} \times (2.29 + F_c)$
	$F_c=(F_d+F_p)F_m$; F_m=3.75; F_d=1.35(kettle reboiler);
	F_d=0.8(for the fixed tubesheet heat exchanges); F_p = 0
Compressor cost	$\frac{M\&S}{280} \times 1609.425 \times (\frac{h_p}{0.8})^{0.82}$
Electricity cost/($ GJ^{-1})	$(\frac{W_{comp} \times C_e}{\eta_m \times \eta_c}) \times 8000$
	C_e = 0.084 $/(kW h)
Energy cost/$	LP steam (433 K) = 7.72 $/GJ
	Cooling water (305 K) = 0.354 $/GJ
	Refrigerant (253 K) = 7.89 $/GJ
Heat transfer coefficients	Condensers 0.852 kW/(K m^2)
	Reboilers 0.568 kW/(K m^2)
	Economizers 0.568 kW/(K m^2)
Marshall & Swift index (M&S)	1431.7 (data from CEPCI)

Notation

N_T	total tray stages	D/m	column diameter
H/m	column height	A/m^2	heat exchanger area
h_p/kW	input horsepower of compressor	W_{comp}/kW	output work of compressor
η_m	motor efficiency (0.9)	η_c	compressor efficiency (0.8)
F_c	capital charge factor	F_p	pressure coefficient

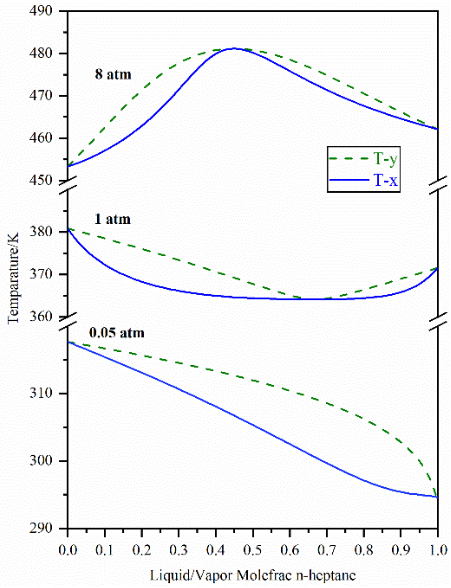

Fig. S1 *T-xy* diagrams for *n*-heptane and isobutanol system at different pressures [4,5].

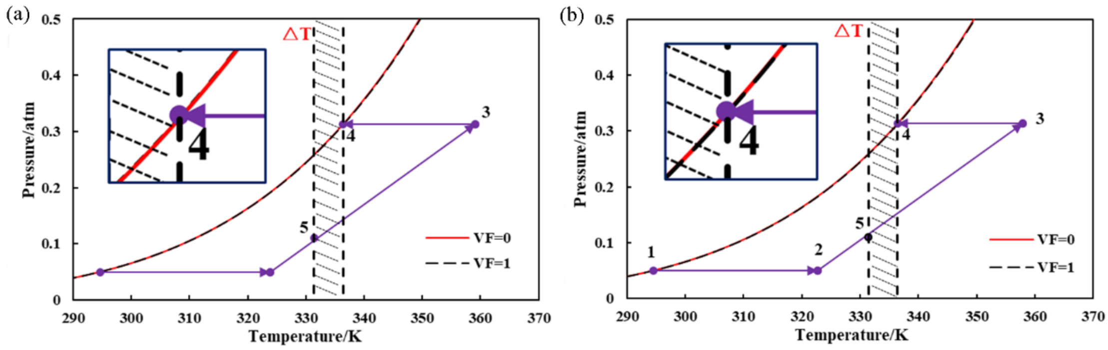

Fig. S2 P-T curves for overhead vapor heat transferring steps: (a) LPVRC; (b) HPVRC.

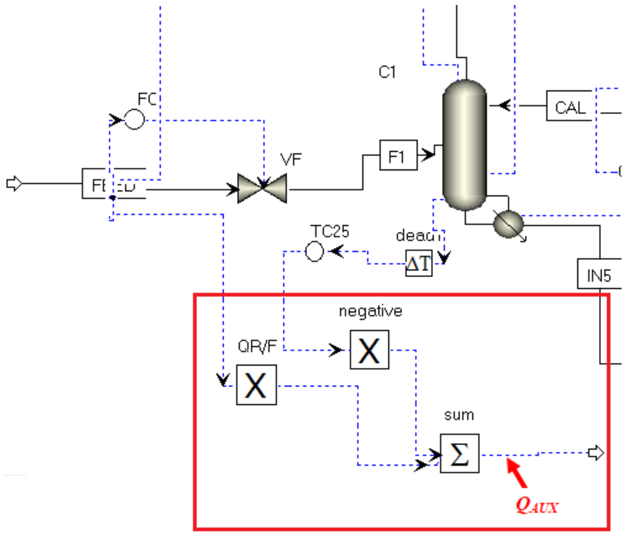

Fig. S3 Aspen Dynamics implementation procedures for the feedforward action by the manipulation of the auxiliary reboiler heat duty Q_{AUX}.

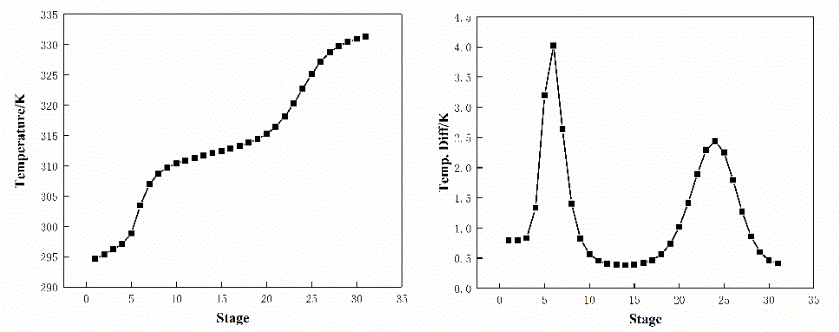

Fig. S4 Temperature and temperature difference profiles.

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Constraints-Flowsheet
CONSTRAINTS
  //Flowsheet variables and equations...
 //The calculation of the virtual heat exchanger REB1 load
 dt1 as temperature;
 dt2 as temperature;
 dt1m as temperature;
 dt1=blocks("COMP").Tout–blocks("C1").stage(31).T;
 dt2=blocks("REB").T–blocks("C1").Stage(31).T;
 dt1m=(dt1-dt2)/loge(dt1/dt2);
 blocks("REB").QR=-0.568*(5.4856/1523.8)*132.483*dt1m;
 //The calculation of the reboiler heat duty for column C1
 blocks("C1").QReb=-blocks("REB").QR+block("sum").Output.;
END
```

Fig. S5 The heat transfer relationship for the intensified configuration.

References

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4. Wang Y, Zhang Z, Xu D, et al. Design and control of pressure-swing distillation for azeotropes with different types of boiling behavior at different pressures. Journal of Process Control, 2016, 42: 59-76

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