SUPPORTING INFORMATION

Operation of a DWDC Separating an Ideal Ternary Mixture of Hypothetical Components, A, B, and C with the SDTDC Scheme

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1. Problem Description and Process Design

The vapor-liquid equilibrium relationship of the hypothetical ternary mixture is expressed by

$P_{j} = x_{A,j} P_{A}^{s} + x_{B,j} P_{B}^{s} + x_{C,j} P_{C}^{s}$	$1 \leq j \leq N$	(1)
$y_{i,j} = x_{i,j} P_{i,j}^s / P_j$	$i = A, B, C, and 1 \le j \le N$	(2)

The vapor saturation pressure can be estimated with the following equation

$$lnP_{i,j}^{s} = A_{vp,i} - B_{vp,i} / T_{j} \qquad i = A, B, C, \text{ and } 1 \le j \le N$$

$$(3)$$

Table 1. Operating Conditions and Design Specifications for the DWDC

Parameter		Value
Condenser pressure (bar)		3
Stage pressure drop (bar)		6.8901×10^{-3}
	А	33.33
Feed compositions (mol %)	В	33.33
	С	33.34
Feed flow rate (kmol/s)		1
Feed thermal condition (liquid fraction	1	
Relative volatility A:B:C	4:2:1	
	$A(A_{vp}/B_{vp})$	13.04/3862
Vapor pressure constants	$B(A_{vp}/B_{vp})$	12.34/3862
	$C(A_{vp}/B_{vp})$	11.65/3862
	А	99
Product specifications (mol %)	В	99
	С	99

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Table 1 summarizes the operating conditions and design specifications for the DWDC to be developed. The commercial software Aspen Plus is used to perform steady-state simulation. A stripping distillation column with only a reboiler, two paralleled absorber distillation columns with neither reboiler nor condenser, and a rectifying distillation column with only a condenser are employed to construct the DWDC. The design of the DWDC is conducted via a simple search procedure proposed in our earlier work and the minimization of total annual cost is chosen as the objective function for process screening. The resultant DWDC is sketched in Figure 1a.



Figure 1. Optimum design of the DWDC and its control schemes: (a) DWDC scheme, (b) TDC scheme, (c) DTDC scheme, (d) SDTDC scheme.

2. Closed-Loop Evaluations of the SDTDC Proposed

Dynamic operations of the DWDC, controlled, respectively, with the TDC, DTDC, and SDTDC schemes, are examined here with the commercial software Aspen Dynamics. The detailed configurations for the TDC/DTDC/SDTDC

scheme are shown, respectively, in Figures 1b to 1d. All temperature sensors contain a 1-min measurement delay and the temperature related control loops are tuned with the built-in Tyreus-Luyben rule. The detailed parameters are summarized in Table 2.

Scheme	Controller	Manipulated variable	Controlled variable	K _C (–)	T _I (min)
TDC	TDC1	D	$T_{10} - T_{p18}$	0.279	14.520
	TDC2	Ι	$T_{35} - T_{26}$	0.745	17.160
	TDC3	Q _R	$T_{46} - T_{40}$	0.365	10.560
	TDC4	R_L	$T_{P22} - T_{P14}$	0.524	19.800
	DTDC1	D	$(T_2 - T_{10}) - (T_{10} - T_{P18})$	0.123	14.520
DTDC	DTDC2	Ι	$(T_{21} - T_{35}) - (T_{35} - T_{39})$	0.202	17.160
	DTDC3	Q _R	$(T_{40} - T_{46}) - (T_{46} - T_{52})$	0.040	10.560
	DTDC4	R_L	$(T_{P14} - T_{P22}) - (T_{P22} - T_{P30})$	0.700	19.800
SDTDC	TC1	D	T ₁₀	3.703	14.520
	DTDC1	Ι	$(T_{21} - T_{35}) - (T_{35} - T_{39})$	0.189	18.480
	TC2	Q _R	T ₄₆	3.612	7.920
	DTDC2	R_L	$(T_{P14} - T_{P22}) - (T_{P22} - T_{P30})$	0.706	21.120
SDTDC-FR	TDC1	D	$T_{P14} - T_{10}$	0.233	13.200
	DTDC1	Ι	$(T_{21} - T_{35}) - (T_{35} - T_{39})$	0.192	17.160
	TDC2	Q _R	$T_{39} - T_{46}$	0.337	10.560
	DTDC2	R_L	$(T_{P14} - T_{P22}) - (T_{P22} - T_{P30})$	0.619	21.120

Table 2. Controller Parameters for the TDC, DTDC, SDTDC and SDTDC-FR Schemes

The closed-loop responses of the DWDC, controlled with the SDTDC scheme, are given in Figure 2 after it has been subjected to a ± 10 % step change in feed compositions of component A. The ratio between feed compositions of components B and C is kept unchanged. Stable regulations of the DWDC are achieved with rather small peak deviations and settling times. The comparisons between the DWDCs, controlled, respectively, with the TDC, DTDC, and SDTDC schemes, are presented in Figure 3, after the processes have been subjected to a ± 10 % step change in feed compositions of components A, B, and C. While the dark lines indicate the responses to the positive step variations in the steady-state operating conditions, the grey lines the responses to the negative step variations in the steady-state operating conditions. Similar settling times are displayed between these three control schemes. In comparison with the TDC scheme, the SDTDC scheme displays reduced steady-state offsets in the intermediate product but slightly amplifiedones in the top and bottom products. As compared with the DTDC scheme, the SDTDC scheme leads to almost the same steady-state offsets in the

intermediate product but slightly amplifiedones in the top and bottom products. In Table 3, the relative steady-state offsets in the three products are tabulated. The TDC scheme maintains the three products within the range of 99 % \pm 0.466 %, the DTDC scheme within the range of 99 % \pm 0.078 %, and the SDTDC scheme within the range of 99 % \pm 0.266 %.





Figure 2. Regulatory responses of the SDTDC in the face of a ±10 % step change in feed compositions of component

A.

Figure 3. Comparison of the regulatory responses of the TDC, DTDC, and SDTDC schemes for a ±10 % step change in feed compositions of components A, B, and C: (a) component A, (b) component B, (c) component C.

Scenario	Decidence]	Relative error (%)			
	FIGUUCI	TDC	DTDC	SDTDC	SDTDC-FR	
+10 % Z _A	А	0.053	0.015	0.056	-0.021	
	В	0.266	0.055	0.051	0.060	
	С	0.091	-0.046	-0.167	0.095	
	А	-0.099	-0.009	-0.059	0.023	
-10 % $Z_{\rm A}$	В	-0.466	-0.046	-0.042	-0.050	
	С	-0.069	0.052	0.142	-0.062	
	А	0.073	-0.046	-0.266	0.127	
+10 % Z _B	В	-0.215	-0.030	-0.022	-0.040	
	С	-0.030	0.016	0.054	-0.041	
-10 % Z _B	А	-0.057	0.078	0.206	-0.086	
	В	0.153	0.065	0.051	0.077	
	С	0.029	-0.014	-0.050	0.042	
+10 % Z _C	А	-0.138	0.062	0.157	-0.069	
	В	-0.190	0.008	0.001	0.017	
	С	-0.046	0.034	0.095	-0.030	
-10 % Z _C	А	0.133	-0.045	-0.202	0.095	
	В	0.133	0.014	0.017	0.007	
	С	0.056	-0.034	-0.108	0.042	

Table 3. Relative Steady-State Errors in the Three Products for a ±10 % Step Change in Feed Compositions of

Components A, B, and C

In Figure 4, the closed-loop responses of the DWDC, controlled with the SDTDC scheme, are shown after it has been subjected to a ± 30 % step change in feed compositions of component A. The ratio between feed compositions of components B and C is kept unchanged. Stable regulations are again achieved but with a certain extent of increased peak deviations and settling times in comparison with those of Figure 2. In Figure 5, the comparisons between the DWDCs, controlled, respectively, with the TDC, DTDC, and SDTDC schemes are detailed after the processes have been subjected to a ± 30 % step change in feed compositions of components A, B, and C. It is noted that the TDC scheme is now unable to suppress the disturbances in the cases of negative change in feed compositions of component A and positive change in feed compositions of components B and C, and gives great sudden drops, respectively, in the top and intermediate products, intermediate and bottom products, and intermediate product. The DTDC and SDTDC schemes can, however, still do a good job and maintain stable operations of the DWDC. In the other circumstances, analogous observations to those

obtained in Figure 3 can again be reached on the SDTDC scheme when compared with the TDC and DTDC schemes. Table 4 summarizes the relative steady-state offsets in the three products. While the TDC and DTDC schemes keep the three products within the range of 99 % \pm 24.869 % and 99 % \pm 0.258 %, respectively, the SDTDC scheme within the range of 99 % \pm 0.895 %.





Figure 4. Regulatory responses of the SDTDC scheme for a ±30 % step change in feed compositions of component

Α.



Figure 5. Comparison of the regulatory responses of the TDC, DTDC, and SDTDC schemes for a ±30 % step change in feed compositions of components A, B, and C: (a) component A, (b) component B, (c) component C.

Scenario	Product	Relative Error (%)			
		TDC	DTDC	SDTDC	SDTDC-FR
+30 % Z _A	А	0.101	0.058	0.159	-0.064
	В	0.579	0.184	0.168	0.219
	С	0.373	-0.113	-0.602	0.485
$-30 \% Z_{A}$	А	-5.479	-0.002	-0.183	0.090
	В	-19.541	-0.103	-0.092	-0.112
	С	-0.164	0.166	0.367	-0.115
	А	0.000	0.105	-0.895	0.564
$+30$ % $Z_{\rm B}$	В	-24.869	-0.258	-0.198	-0.349
	С	-3.842	0.053	0.185	-0.140
-30 % Z_B	А	-0.137	0.251	0.485	-0.182
	В	0.365	0.241	0.191	0.278
	С	0.082	-0.035	-0.136	0.127
+30 % Z _C	А	-0.501	0.197	0.381	-0.145
	В	-1.100	0.084	0.049	0.104
	С	-0.105	0.108	0.257	-0.058
-30 % Z _C	А	0.417	-0.005	-0.791	0.394
	В	0.272	0.018	-0.034	0.035
	С	0.221	-0.105	-0.361	0.167

Table 4. Relative Steady-State Errors in the Three Product Qualities for a ±30 % Step Change in Feed Compositions

of Components A, B, and C

3. Further Reinforcement of the SDTDC Proposed

The SDTDC scheme can be further reinforced through the formation of 1 or 2 TDC loops in the rectifying and/or stripping sections with the available temperature measurements in the two sections along the dividing wall. One of the schemes (i.e., the SDTDC–FR scheme) is found effective for the DWDC studied and sketched in Figure 6. The SDTDC–FR scheme forms 2 TDC loop with the top/bottom temperature measurement in the left/right side of the dividing wall (indicated here by the bold dashed lines). The temperature related controllers are retuned and the resultant parameters are also tabulated in Tables 2. Figure 7 depicts the closed-loop responses of the DWDC, controlled with the SDTDC and SDTDC–FR schemes, after encountering a ± 30 % step change in feed compositions of components A, B, and C. It is straightforward to notice that the SDTDC–FR scheme is advantageous over the SDTDC scheme, especially in the steady-state offsets of the top and bottom products. The relative steady-state offsets of the SDTDC–FR schemes are also

given in Table 4.



Figure 6. Further reinforcement of the SDTDC scheme (SDTDC-FR).



Figure 7. Comparison of the SDTDC and SDTDC-FR schemes for a ±30 % step change in feed compositions of components A, B, and C: (a) component A, (b) component B, (c) component C.