

Electronic Supplementary Material

Determination of a suitable index for a solvent via two-column extractive distillation using a heuristic method

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List of table captions

Table S1. The binary interaction parameters of toluene-methanol.

Table S2. The binary interaction parameters of acetone-methanol.

List of Figure captions

Fig. S1. The flowsheet information with NMP as entrainer.

Fig. S2. The flowsheet information with aniline as entrainer.

Fig. S3. The flowsheet information with N,N-dimethylacetamide as entrainer.

Fig. S4. The flowsheet information with styrene as entrainer.

Fig. S5. The flowsheet information with o-xylene as entrainer.

Fig. S6. The flowsheet information with m-xylene as entrainer.

Fig. S7. The flowsheet information with p-xylene as entrainer.

Fig. S8. The flowsheet information with MEA as entrainer.

Fig. S9. The flowsheet information with Water as entrainer.

Fig. S10. The flowsheet information with Ethanol as entrainer.

Fig. S11. The flowsheet information with DMSO as entrainer.

Fig. S12. The flowsheet information with DMF as entrainer.

Table S1. The binary interaction parameters of toluene-methanol.

Component.i	Toluene	Toluene	Methanol	Toluene	Methanol	Toluene	Methanol	Toluene	Methanol	Toluene	Methanol	Toluene	Methanol	Toluene	Methanol	
Component.j	Methanol	NMP	NMP	Aniline	Aniline	C4H9NO	C4H9NO	Styrene	Styrene	o-xylene	o-xylene	p-xylene	p-xylene	m-xylene	m-xylene	
Source	AVP72 VLE-IG	AVP72 VLE-IG	R-PCES	AVP72 VLE-IG	AVP72 VLE-IG	R-PCES	R-PCES	R-PCES	R-PCES	R-PCES	R-PCES	AVP72 VLE-IG	AVP72 VLE-IG	AVP72 VLE-IG	AVP72 VLE-IG	
A _{ij}	0.0	0.4132	0.0	0.9547	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.5285	0.0	0.0	
A _{ji}	0.0	-0.5048	0.0	-0.3418	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.3930	0.0	0.0	
B _{ij}	-563.01	-44.826	54.436	-435.76	88.414	4.1403	37.355	-563.01	54.436	-13.344	40.331	24.560	247.46	151.33	37.758	
B _{ji}	27.831	171.516	-60.116	110.26	-291.40	41.595	-66.675	27.831	-60.116	14.081	-606.05	-20.761	-1511.5	-235.89	-609.38	
C _{ij}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
C _{ji}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
D _{ij}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
D _{ji}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
E _{ij}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
E _{ji}	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
TLOWER	336.65	363.25	298.15	313.15	293.15	298.15	298.15	336.65	298.15	298.15	298.15	298.15	384.38	313.15	383.730	337.80
TUPPER	383.75	436.85	298.15	427.05	338.15	298.15	298.15	383.75	298.15	298.15	298.15	298.15	410.25	411.45	412.290	412.15

Table S2. The binary interaction parameters of acetone-methanol.

Component.i	Methanol	Acetone	Methanol	Methanol	Acetone	Methanol	Acetone	Methanol	Acetone	Methanol	Acetone	Methanol	Acetone
Component.j	Acetone	Water	Water	MEA	MEA	EG	EG	DMSO	DMSO	DMF	DMF	Ethanol	Ethanol
Source	AVP72 VLE-IG	AVP72 VLE-IG	APV72 VLE-IG	R-PCES	R-PCES	AVP72 VLE-IG	AVP72 VLE-IG	AVP72 VLE-IG	AVP72 VLE-IG	APV72 VLE-IG	APV72 VLE-IG	APV72 VLE-IG	AVP72 VLE-IG
A _{ij}	0	6.3981	-0.693	0	0	33.3298	0	0	0	-0.703	0	4.7119	-0.3471
A _{ji}	0	0.0544	2.7322	0	0	0.1753	0	0	0	1.1467	0	-2.3127	-1.0787
B _{ij}	114.13	-1808.99	172.99	-1050.5	599.61	-10000	386.73	30.5966	167.14	301.44	-17.224	-1162.3	206.59
B _{ji}	101.88	419.971	-617.27	2751.9	-98.522	-322.92	236.85	-331.16	39.842	-400.24	-5.1717	483.84	479.05
C _{ij}	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0.3	0	0	0.3	0.3
C _{ji}	0	0	0	0	0	0	0	0	0	0	0	0	0
D _{ij}	0	0	0	0	0	0	0	0	0	0	0	0	0
D _{ji}	0	0	0	0	0	0	0	0	0	0	0	0	0
E _{ij}	0	0	0	0	0	0	0	0	0	20	20	0	0
E _{ji}	0	0	0	0	0	0	0	0	0	152.5	152.9	0	0
TLOWER	55	20	24.99	25	25	40	50	20	25	0	0	20	25
TUPPER	64.65	95.1	100	25	25	199	50	40	45	0	0	78.4	78.3

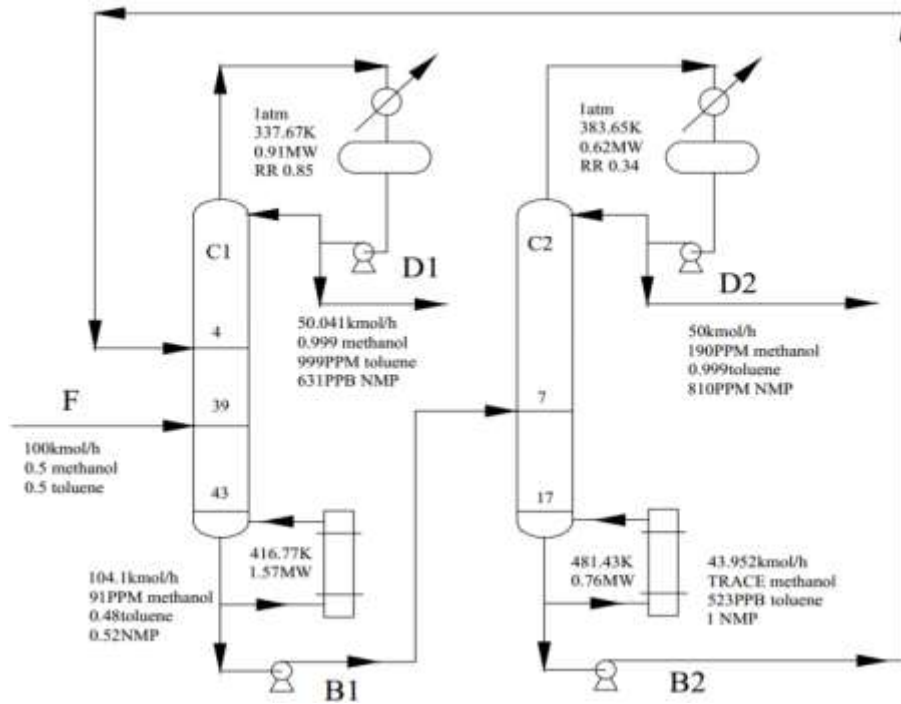


Figure S1. The flowsheet information with NMP as entrainer

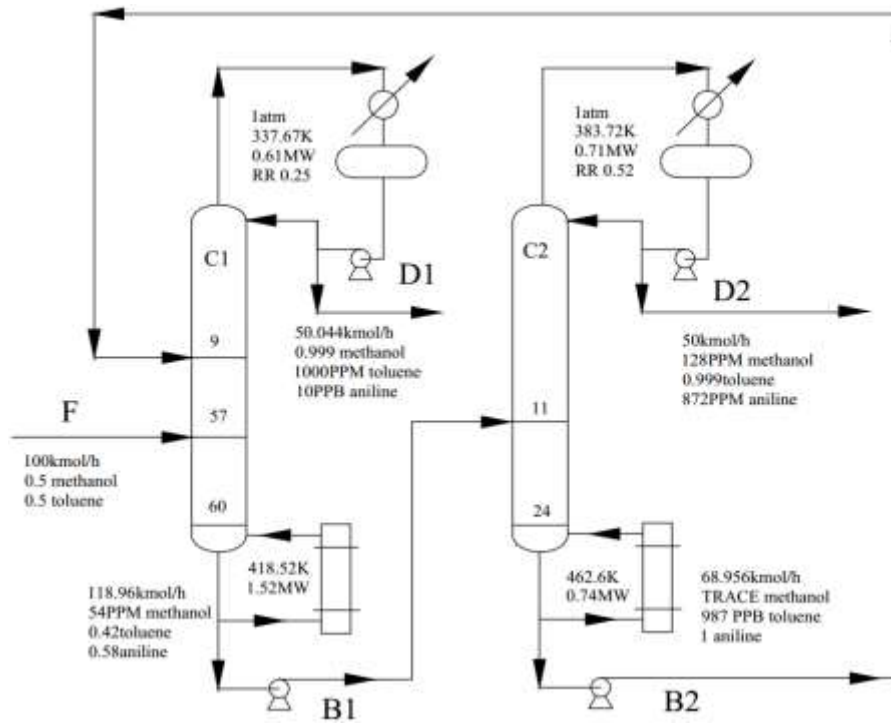


Figure S2. The flowsheet information with aniline as entrainer

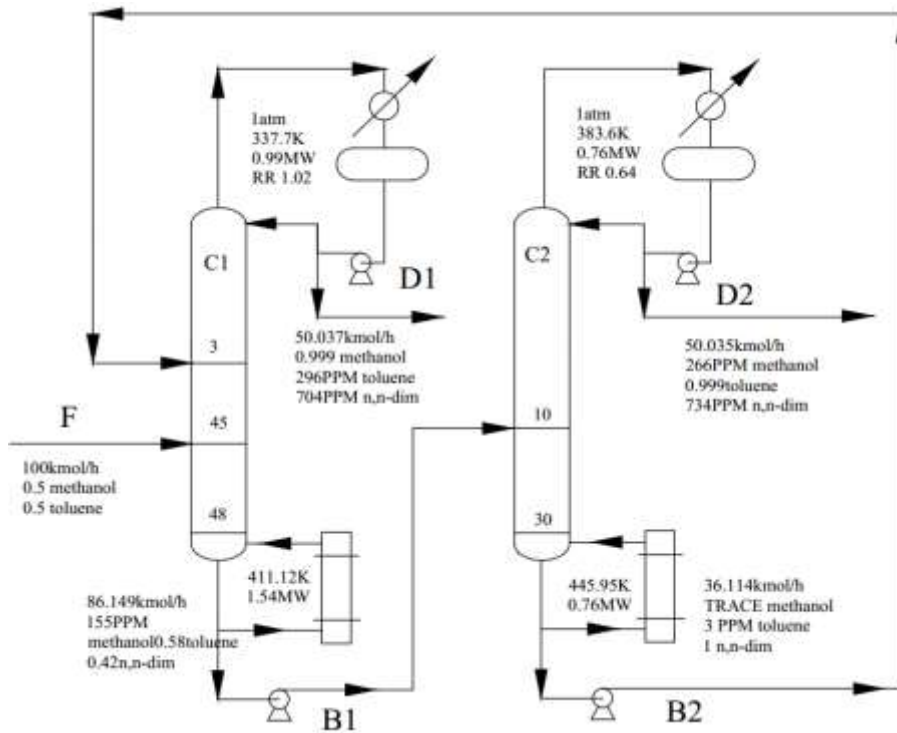


Figure S3. The flowsheet information with N,N-dimethylacetamide as entrainer

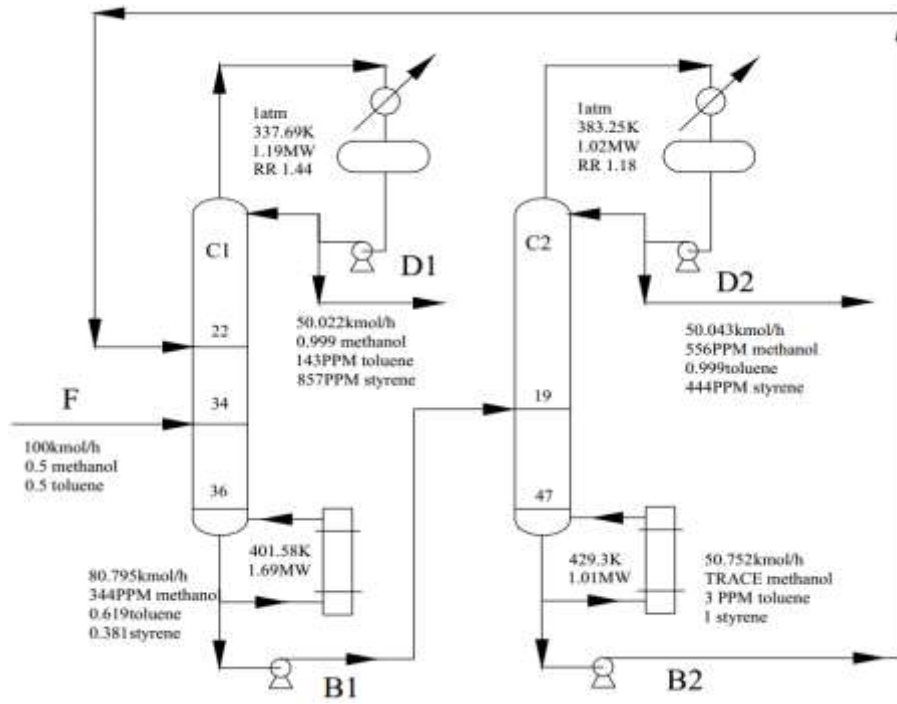


Figure S4. The flowsheet information with styrene as entrainer

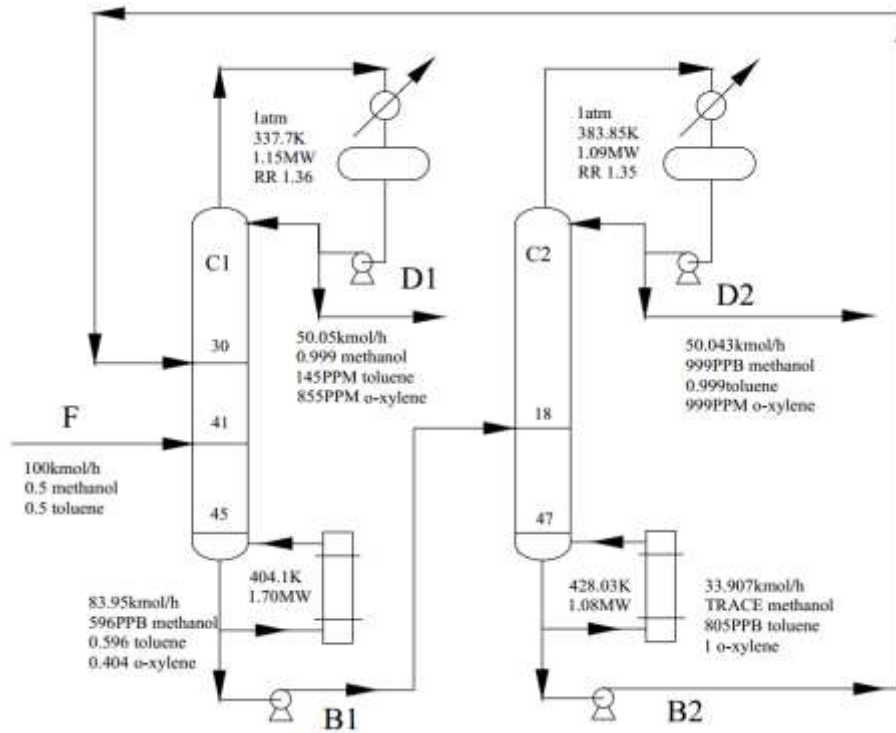


Figure S5. The flowsheet information with o-xylene as entrainer

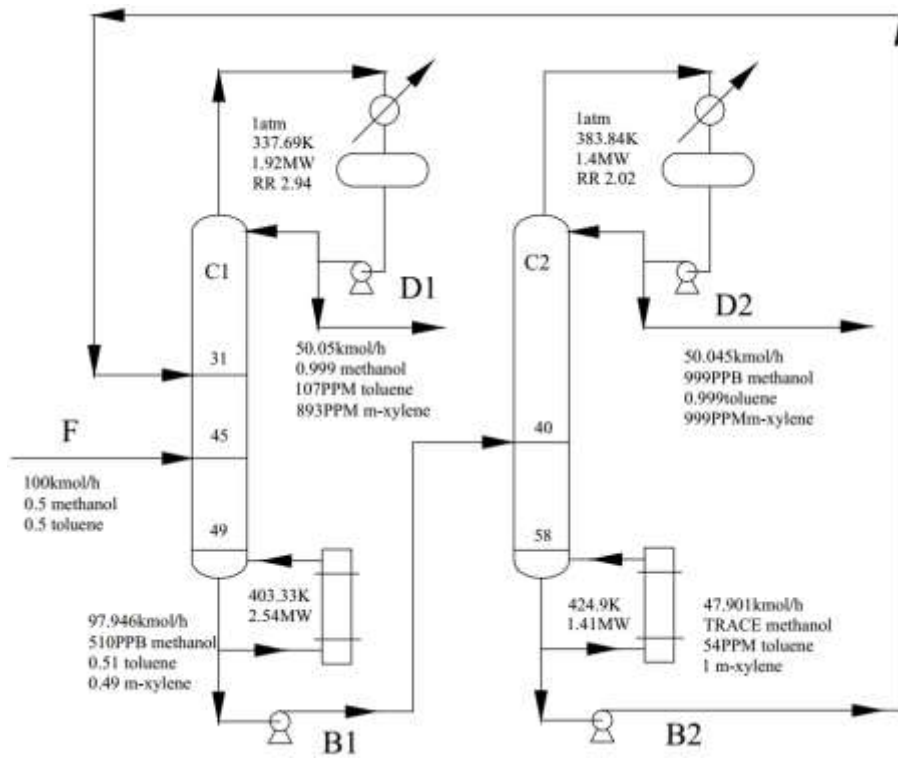


Figure S6. The flowsheet information with m-xylene as entrainer

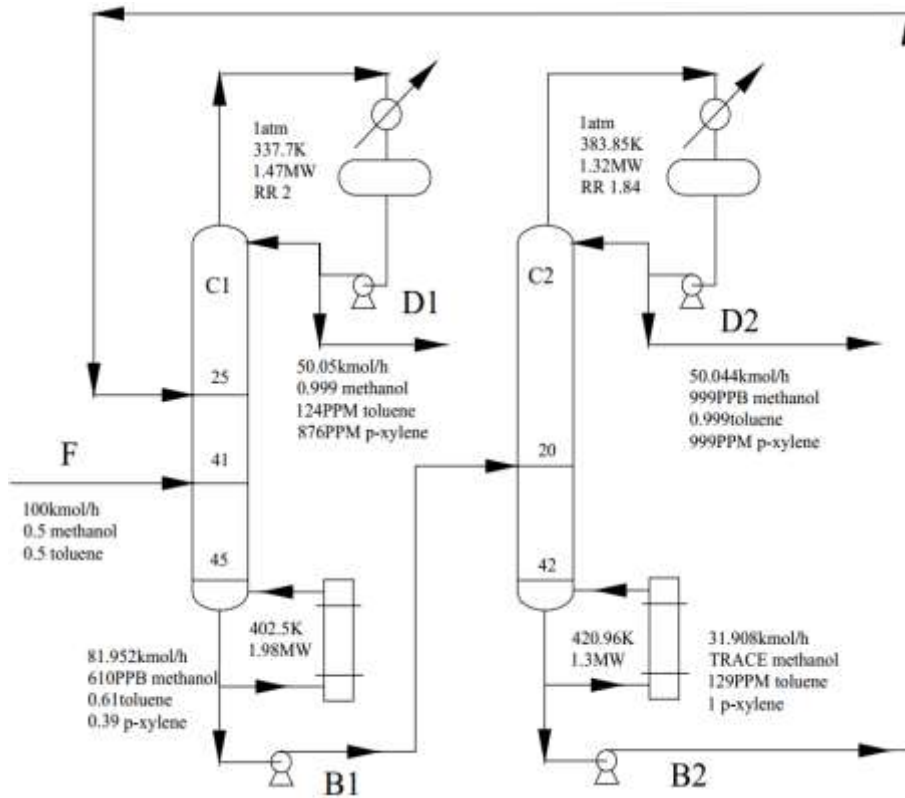


Figure S7. The flowsheet information with p-xylene as entrainer

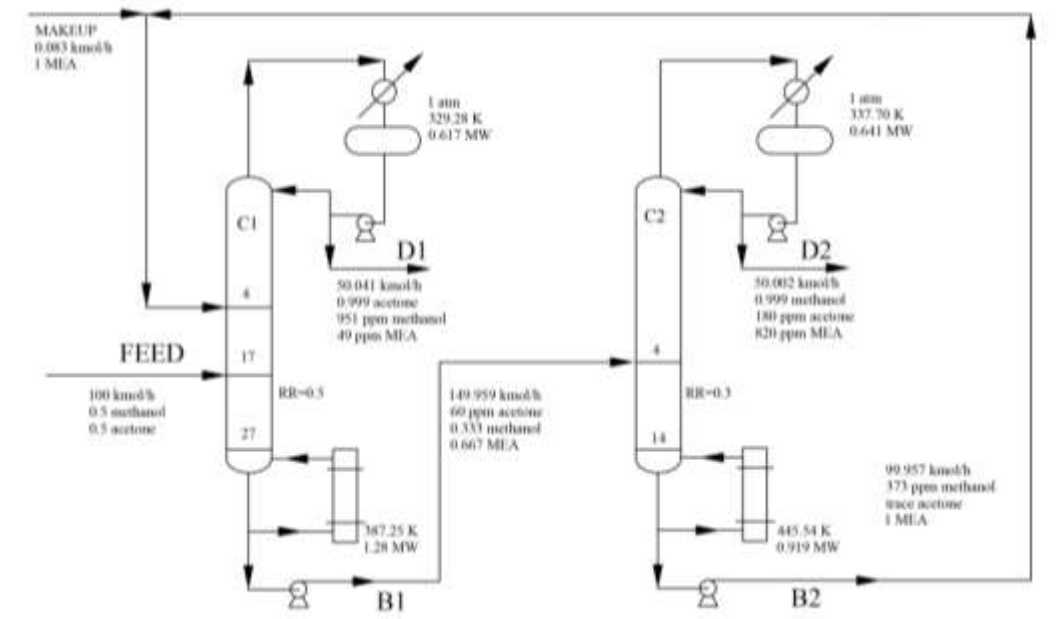


Figure S8. The flowsheet information with MEA as entrainer

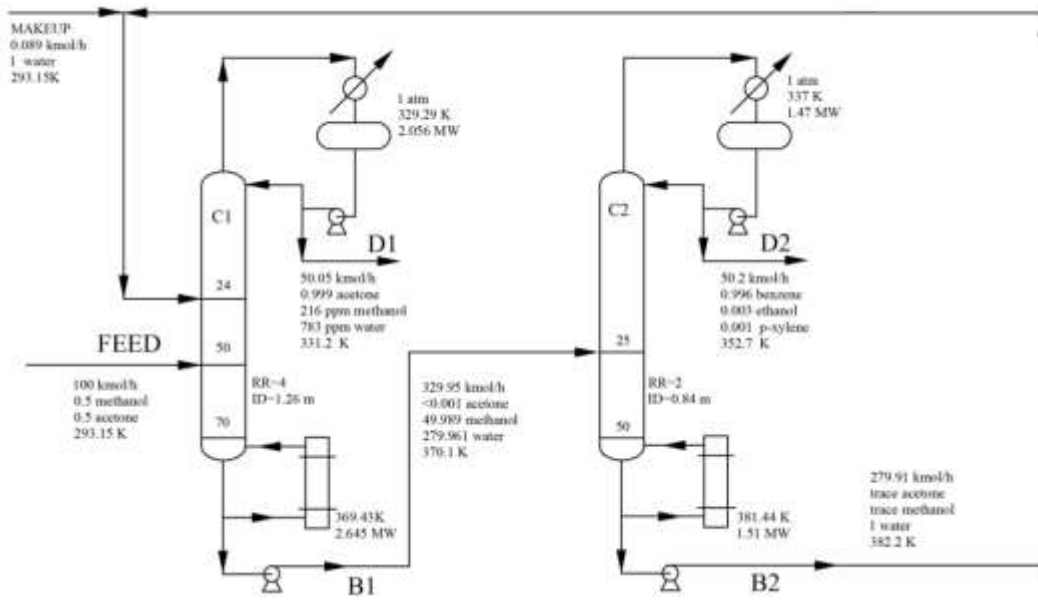


Figure S9. The flowsheet information with Water as entrainer

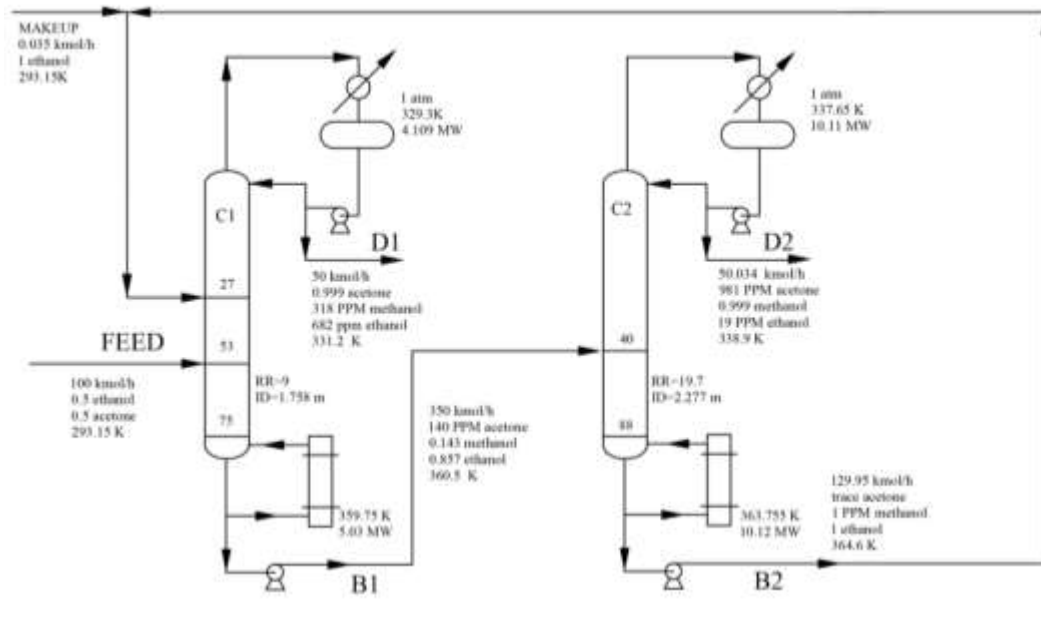


Figure S10. The flowsheet information with Ethanol as entrainer

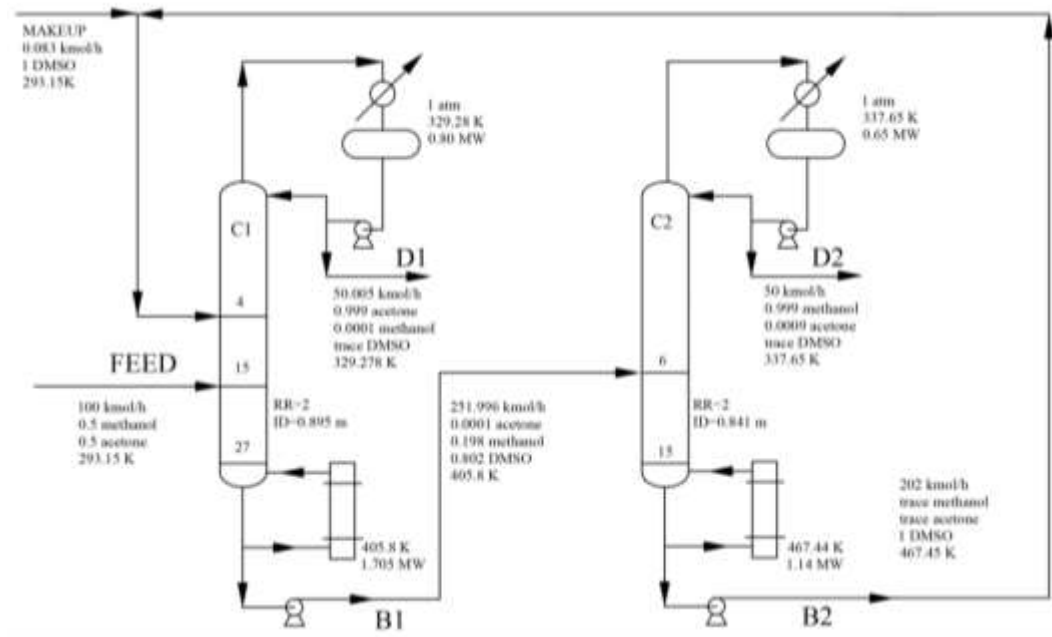


Figure S11. The flowsheet information with DMSO as entrainer

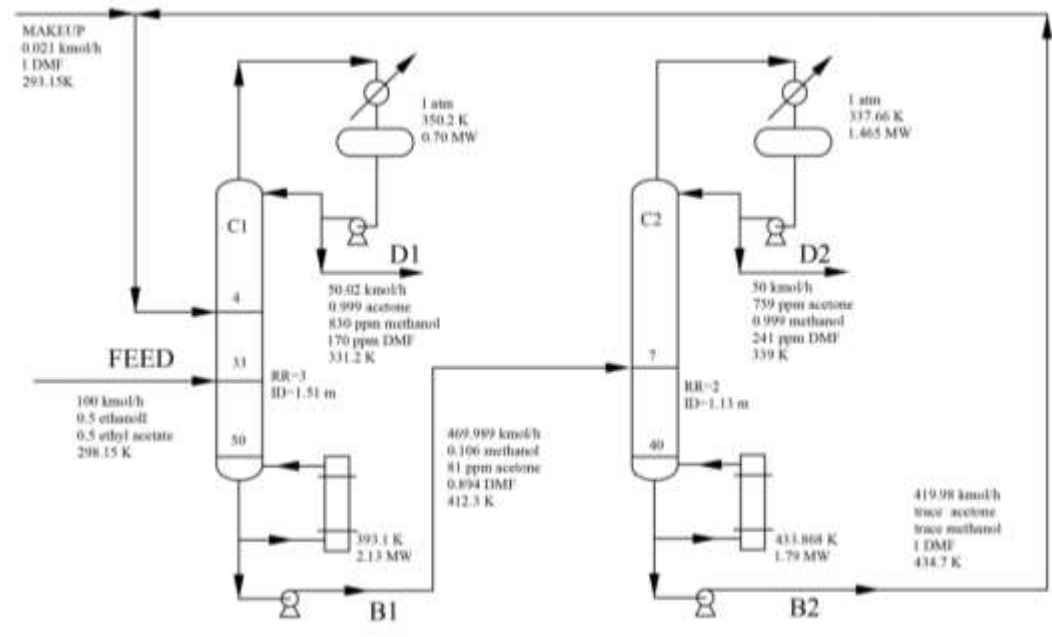


Figure S12. The flowsheet information with DMF as entrainer