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APPENDICES

Appendix A Solubility Parameter (δ_{IL}) Values of Ionic Liquids

Experimental values for 39 different ionic liquids at 298.15 K were used for the development of the Hildebrand solubility parameter GC model (Marciniak, 2010, Marciniak, 2011, Weerachanchai *et al.*, 2012, Yoo *et al.*, 2012). The total numbers of independent variables in the model are 34 (including a constant term). The developed model (see Equation (4.1) provides a good fit of experimental data with a value of 0.319%AARD between the predicted and experimental solubility parameter values. The maximum relative deviation observed was 3.29.

Table A1 The experimental and predicted solubility parameter (δ_{IL}) values of ionic liquids

No.	Ionic liquid	Abbreviation	δ_{IL}/MPa$^{0.5}$ (Exp)	δ_{IL}/MPa$^{0.5}$ (Calc)	RD	%AARD	References
1	1-Ethyl-3-methyl-imidazolium trifluoroacetate	[C2mim][CF3COO]	25.56	25.56	0.000	0.000	Marciniak et al. (2010)
2	1-(3-hydroxypropyl)pyridinium bis(trifluoromethylsulfonyl)imide	[N-C3OHPY][Tf2N]**	26.00	26.00	0.000	0.000	Marciniak et al. (2011)
3	1-(3-hydroxypropyl)pyridinium trifluorotris(perfluoroethyl)phosphate	[N-C3OHPY][FAP]**	25.00	25.00	0.000	0.000	Marciniak et al. (2011)
4	1,3-Dihexyloxymethyl-imidazolium bis(trifluoromethylsulfonyl)imide	[(C6OC)2im][Tf2N]	19.60	19.60	0.000	0.000	Marciniak et al. (2010)
5	1,3-dimethylimidazolium dimethylphosphate	[C1mim][DMP]*	27.08	27.08	0.000	0.000	Marciniak et al. (2010)
6	1,3-Dimethylimidazolium methylsulfate	[C1mim][MeSO4]	26.36	26.36	0.000	0.000	Piyarat et al. (2012)
7	1-butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide	[C4mPip][Tf2N]*	23.40	23.40	0.003	0.000	Marciniak et al. (2011)
8	1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	[C_4mpyr][Tf_2N]	25.81	25.88	0.067	0.007	Piyarat et al. (2012)
9	1-butyl-1-methylpyrrolidinium dicyanamide	[C_4mpyr][N$(CN)_2$]	25.54	25.54	0.000	0.000	Piyarat et al. (2012)
10	1-butyl-1-methylpyrrolidinium thiocyanate	[C_4mpyr][SCN]	24.96	24.89	0.073	0.008	Marciniak et al. (2010)
11	1-butyl-1-methylpyrrolidinium trifluoromethanesulfonate	[C_4mpyr][CF_3SO_3]	22.83	22.83	0.000	0.000	Marciniak et al. (2010)

Table A1 The experimental and predicted solubility parameter (δ_{IL}) values of ionic liquids (Continued)

No.	Ionic liquid	Abbreviation	δ_{IL}/MPa$^{0.5}$ (Exp)	δ_{IL}/MPa$^{0.5}$ (Calc)	RD	%AARD	References
12	1-Butyl-3-methyl-midazolium 2-(2-methoxyethoxy)ethyl sulfate	$[C_4mim][MDEGSO_4]$	24.80	24.80	0.000	0.000	Marciniak et al. (2010)
13	1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	$[C_4mim][Tf_2N]$	25.69	25.71	0.016	0.002	Piyarat et al. (2012)
14	1-Butyl-3-methylimidazolium chloride	$[C_4mim][Cl]$	24.14	24.14	0.000	0.000	Piyarat et al. (2012)
15	1-butyl-3-methylimidazolium hexafluoroantimonate	$[C_4mim][SbF_6]$	31.50	31.50	0.000	0.000	Marciniak et al. (2010)
16	1-Butyl-3-methyl-imidazolium octyl sulfate	$[C_4mim][OcSO_4]$	24.80	24.80	0.000	0.000	Marciniak et al. (2010)
17	1-Butyl-3-methyl-imidazolium thiocyanate	$[C_4mim][SCN]$	24.64	24.72	0.075	0.008	Marciniak et al. (2010)
18	1-Butyl-3-methyl-imidazolium trifluoromethanesulfonate	$[C_4mim][CF_3SO_3]$	22.67	22.66	0.010	0.001	Marciniak et al. (2010)
19	1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	$[C_4mim][Tf_2N]$	26.70	25.71	0.994	0.095	Marciniak et al. (2010)
20	1-Butyl-3-methylpyridinium trifluoromethanesulfonate	$[C_4mpy][CF_3SO_3]$	22.47	22.47	0.000	0.000	Marciniak et al. (2010)
21	1-Butyl-4-methylpyridinium thiocyanate	$[_{1,4}bmPY][SCN]$	24.53	24.53	0.003	0.000	Marciniak et al. (2010)
22	1-Butyl-4-methylpyridinium tosylate	$[_{1,4}bmPY][TOS]$	23.06	23.06	0.000	0.000	Marciniak et al. (2010)

Table A1 The experimental and predicted solubility parameter (δ_{IL}) values of ionic liquids (Continued)

No.	Ionic liquid	Abbreviation	δ_{IL}/MPa$^{0.5}$ (Exp)	δ_{IL}/MPa$^{0.5}$ (Calc)	RD	%AARD	References
25	1-Ethyl-3-methylimidazolium acetate	[C_2mim][Ac]	25.16	25.16	0.000	0.000	Piyarat et al. (2012)
26	1-ethyl-3-methylimidazolium tetracyanoborate	[C_2mim][TCB]	25.90	25.90	0.000	0.000	Marciniak et al. (2011)
27	1-Ethyl-3-methyl-imidazolium thiocyanate	[C_2mim][SCN]	25.19	25.19	0.000	0.000	Marciniak et al. (2010)
28	1-hexyl-3-methylimidazolium hexafluorophosphate	[C_6mim][PF_6]	28.60	28.60	0.000	0.000	Marciniak et al. (2010)
29	1-Hexyl-3-methyl-imidazolium thiocyanate	[C_6mim][SCN]	23.65	24.24	0.590	0.064	Marciniak et al. (2010)
30	1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	[C_8mim][Tf_2N]	25.00	24.76	0.244	0.025	Marciniak et al. (2010)
31	1-methyl-3-octylimidazolium hexafluorophosphate	[C_8mim][PF_6]	27.80	28.13	0.325	0.030	Marciniak et al. (2010)
32	1-propyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide	[C_3mPip][Tf_2N]*	23.80	23.64	0.159	0.017	Marciniak et al. (2011)
33	N-octyl-isoquinolinium bis(trifluoromethylsulfonyl)imide	[C_8isoq][NTf_2]*	22.50	22.50	0.000	0.000	Marciniak et al. (2011)
34	Triethyl-sulfonium bis(trifluoromethylsulfonyl)imide	[Et_3S][NTf_2]	21.05	21.05	0.000	0.000	Marciniak et al. (2010)

Table A1 The experimental and predicted solubility parameter (δ_{IL}) values of ionic liquids (Continued)

No.	Ionic liquid	Abbreviation	δ_{IL}/MPa$^{0.5}$ (Exp)	δ_{IL}/MPa$^{0.5}$ (Calc)	RD	%AARD	References
35	Triisobutyl-methyl-phosphonium tosylate	[P1,i4,i4,i4][TOS]	24.33	24.33	0.000	0.000	Marciniak et al. (2010)
36	Ethylammonium nitrate	[C_2A][NO_3]*	25.17	25.17	0.000	0.000	Yoo et al. (2012)
37	1-ethyl-3-methylimidazolium ethylsulfate	[C_2mim][$EtSO_4$]*	24.45	24.45	0.001	0.000	Yoo et al. (2012)
38	1-Butyl-3-methyl-imidazolium hexafluorophosphate	[C_4mim][PF_6]	29.80	29.07	0.725	0.062	Marciniak et al. (2010)
39	1-Butyl-3-methylimidazolium tetrafluoroborate	[C_4mim][BF_4]	31.60	31.60	0.000	0.000	Marciniak et al. (2010)
				Summation	3.29	0.3197	

*Extrapolated values calculated using linear regression.

**Extrapolated values calculated using polynomial regression.

Appendix B Solubility of ILs and Target Component

The solubility (x_i) of ILs in the target components for poorly miscible liquids can be estimated to the infinite-dilution activity coefficient (Batista *et al.*, 2011) by

$$x_i = \frac{1}{\gamma_i^{\infty}} \quad \text{(B1)}$$

Where, γ_i^{∞} is the infinite-dilution activity coefficient of the component i. The γ_i^{∞} have been taken from the literatures or calculated from predictive thermodynamic models, e.g., UNIFAC models. However, author tried to apply the UNIFAC model for ionic liquids (UNIFAC-IL) proposed by Roughton et al. (2012) for calculation of the γ_i^{∞}, but it could not be accuracy as compared to the experimental data. Therefore, the γ_i^{∞} and/or x_i have been collected from the available literatures as illustrated in Table B1 and B2. It should be noted that the solubility is the mole fraction of the target component divided by the total mole fraction of the mixtures. If the x_i is greater than 1, it means the mixtures are totally soluble.

B.1 The Solubility of ILs and Water (Aqueous Systems)

The experimental mole fraction solubility of the ILs in water (x^{exp}_w) at 298.15 K have been taken from (Klähn *et al.*, 2010, Pereiro *et al.*, 2012) as showed in Table B1.

B.2 The Solubility of ILs and Benzene (Non-Aqueous Systems)

For non-aqueous systems, the infinite-dilution activity coefficient of the benzene (γ_B^{∞}) at 298.15 K have been taken from (Krummen *et al.*, 2002, David *et al.*, 2003, Letcher *et al.*, 2003, Kato and Gmehling, 2005, Foco *et al.*, 2006, Heintz *et al.*, 2006, Domanska and Marciniak, 2007, Mutelet and Jaubert, 2007, Domańska and Marciniak, 2008, Domańska and Laskowska, 2009, Domańska and Królikowski, 2012, Kan *et al.*, 2012, Tumba *et al.*, 2012, Paduszyński and Domańska, 2013) and

the experimental mole fraction solubility of the ILs in benzene (x^{exp}_B) was calculated by Eq. B1. As illustrated in Table B2.

Table B1 The mole fraction solubility of the ILs in water at 298.15 K

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	x^{exp}_{w}	Reference
C8mPy-CF3SO3	3-methyl-1-octylpyridinium trifluoromethanesulfonate	21.52	0.80	Klähn et. al (2010)
C8mim-CF3SO3	1-methyl-3-octylimidazolium trifluoromethanesulfonate	21.71	miscible	Klähn et. al (2010)
C3Pip-Tf2N	1-methyl-1-propylpiperidinium trifluoromethanesulfonate	22.36	0.21	Klähn et. al (2010)
C4mim-CF3SO3	1-butyl-3-methylimidazolium trifluoromethanesulfonate	22.66	miscible	Klähn et. al (2010)
C2eim-CF3SO3	1,3-diethylimidazolium trifluoromethanesulfonate	22.90	miscible	Klähn et. al (2010)
C2mim-CH3SO3	1-ethyl-3-methylimidazolium methanesulfonate	23.14	miscible	Klähn et. al (2010)
C8mim-Cl	1-methyl-3-octylimidazolium chloride	23.19	miscible	Klähn et. al (2010)
C1mim-CF3SO3	1,3-dimethylimidazolium trifluoromethanesulfonate	23.37	miscible	Klähn et. al (2010)
C6mim-Cl	1-hexyl-3-methylimidazolium chloride	23.67	miscible	Klähn et. al (2010)
C4mim-Cl	1-butyl-3-methylimidazolium chloride	24.14	miscible	Klähn et. al (2010)
C2emim-CF3SO3	1-ethyl-2-ethyl-3-methylimidazolium trifluoromethanesulfonate	24.17	miscible	Klähn et. al (2010)
C8mPy-N(CN)2	3-methyl-1-octylpyridinium dicyanamide	24.23	0.95	Klähn et. al (2010)

Table B1 The mole fraction solubility of the ILs in water at 298.15 K (Continued)

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	x^{exp}_{w}	Reference
C2mPy-EtSO4	1-ethyl-3-methylpyridinium ethylsulfate	24.27	miscible	Pereiro et. al (2010)
C2mmim-CF3SO3	1-ethyl-2,3-dimethylimidazolium trifluoromethanesulfonate	24.41	miscible	Klähn et. al (2010)
C8mim-N(CN)2	1-methyl-3-octylimidazolium dicyanamide	24.42	miscible	Klähn et. al (2010)
C2mim-EtSO4	1-ethyl-3-methylimidazolium ethylsulfate	24.45	miscible	Pereiro et. al (2010)
C4mim-Ac	1-butyl-3-methylimidazolium acetate	24.47	miscible	Klähn et. al (2010)
C8Py-Tf2N	1-octylpyridinium bis(trifluoromethylsulfonyl)imide	24.57	0.18	Klähn et. al (2010)
C8mPy-Tf2N	3-methyl-1-octylpyridinium bis(trifluoromethylsulfonyl)imide	24.57	0.16	Klähn et. al (2010)
C2mim-Cl	1-ethyl-3-methylimidazolium chloride	24.61	miscible	Pereiro et. al (2010)
C8mim-Tf2N	1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)imide	24.76	0.19	Klähn et. al (2010)
C4eim-CF3COO	1-butyl-3-ethylimidazolium trifluoroacetate	24.85	miscible	Klähn et. al (2010)
C7mim-Tf2N	1-heptyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	24.99	0.20	Klähn et. al (2010)
C4mim-CF3COO	1-butyl-3-methylimidazolium trifluoroacetate	25.09	miscible	Klähn et. al (2010)

Table B1 The mole fraction solubility of the ILs in water at 298.15 K (Continued)v

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	x^{exp}_{w}	Reference
C2mim-Ac	1-ethyl-3-methylimidazolium acetate	25.16	miscible	Pereiro et. al (2010)
C2mim-SCN	1-ethyl-3-methylimidazolium thiocyanate	25.19	miscible	Klähn et. al (2010)
C6mim-Tf2N	1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	25.23	0.21	Klähn et. al (2010)
C2eim-CF3COO	1,3-diethylimidazolium trifluoroacetate	25.32	miscible	Klähn et. al (2010)
C4mim-N(CN)2	1-butyl-3-methylimidazolium dicyanamide	25.37	miscible	Klähn et. al (2010)
C4eim-Tf2N	1-butyl-3-ethylimidazolium bis(trifluoromethylsulfonyl)imide	25.47	0.24	Klähn et. al (2010)
C5mim-Tf2N	1-methyl-3-pentylimidazolium bis(trifluoromethylsulfonyl)imide	25.47	0.22	Klähn et. al (2010)
C2mim-CF3COO	1-ethyl-3-methylimidazolium trifluoroacetate	25.56	miscible	Klähn et. al (2010)
C4mim-MeSO4	1-butyl-3-methylimidazolium methylsulfate	25.65	miscible	Pereiro et. al (2010)
C4mim-Tf2N	1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	25.71	0.26	Klähn et. al (2010)
C2eim-(Et)2PO4	1,3-diethylimidazolium diethylphosphate	25.72	miscible	Pereiro et. al (2010)
C3mPy-Tf2N	3-methyl-1-propylpyridinium bis(trifluoromethylsulfonyl)imide	25.75	0.24	Klähn et. al (2010)

Table B1 The mole fraction solubility of the ILs in water at 298.15 K (Continued)

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	x^{exp}_{w}	Reference
C1mim-CF3COO	1,3-dimethylimidazolium trifluoroacetate	25.80	miscible	Klähn et. al (2010)
C2mim-N(CN)2	1-ethyl-3-methylimidazolium dicyanamide	25.84	miscible	Klähn et. al (2010)
C4mPyr-TF2N	1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	25.88	0.21	Klähn et. al (2010)
C2eim-Tf2N	1,3-diethylimidazolium bis(trifluoromethylsulfonyl)imide	25.94	0.31	Klähn et. al (2010)
C3mim-Tf2N	1-methyl-3-propylimidazolium bis(trifluoromethylsulfonyl)imide	25.94	0.27	Klähn et. al (2010)
C2mim-(Et)2PO4	1-ethyl-3-methylimidazolium diethylphosphate	25.96	1.00	Pereiro et. al (2010)
C3mPyr-Tf2N	1-methyl-1-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide	26.11	0.23	Klähn et. al (2010)
C2mim-Tf2N	1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	26.18	0.30	Klähn et. al (2010)
C1mim-Tf2N	1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	26.42	0.35	Klähn et. al (2010)
C2mim-DMP	1-ethyl-3-methylimidazolium dimethylphosphate	26.84	miscible	Pereiro et. al (2010)
C2emim-Tf2N	1,2-diethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	27.22	0.28	Klähn et. al (2010)
C2mmim-Tf2N	1-ethyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	27.46	0.33	Klähn et. al (2010)

Table B1 The mole fraction solubility of the ILs in water at 298.15 K (Continued)

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	x^{exp}_{w}	Reference
C8mim-PF6	1-methyl-3-octylimidazolium hexafluorophosphate	28.13	0.21	Klähn et. al (2010)
C6mim-PF6	1-hexyl-3-methylimidazolium hexafluorophosphate	28.60	0.23	Klähn et. al (2010)
C4mim-PF6	1-butyl-3-methylimidazolium hexafluorophosphate	29.07	0.27	Klähn et. al (2010)
C4mmim-PF6	1-butyl-2,3-dimethylimidazolium hexafluorophosphate	30.35	0.22	Klähn et. al (2010)
C8mPy-BF4	3-methyl-1-octylpyridinium tetrafluoroborate	30.46	0.68	Klähn et. al (2010)
C8mim-BF4	1-methyl-3-octylimidazolium tetrafluoroborate	30.65	0.63	Klähn et. al (2010)
C4mim-BF4	1-butyl-3-methylimidazolium tetrafluoroborate	31.60	miscible	Klähn et. al (2010)
C2mim-BF4	1-ethyl-3-methylimidazolium tetrafluoroborate	32.07	miscible	Klähn et. al (2010)

Table B2 The mole fraction solubility of ILs in benzene at 298.15 K

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	γ_B^{∞}	$x^{exp}{}_B$	Reference
C2mim-SCN	1-ethyl-3-methyl-imidazolium thiocyanate	25.19	3.43	0.29	Doman´ska et al. (2008)
C2mim-BF4	1-ethyl-3-methylimidazolium tetrafluoroborate	32.07	2.42*	0.41	Foco et al. (2006)
C4mim-BF4	1-butyl-3-methylimidazolium tetrafluoroborate	31.60	2.39*	0.42	Foco et al. (2006)
C6mim-BF4	1-hexyl-3-methylimidazolium tetrafluoroborate	31.12	1.63*	0.61	Foco et al. (2006)
C8mim-BF4	1-methyl-3-octylimidazolium tetrafluoroborate	30.65	1.28*	0.78	Foco et al. (2006)
C8mim-Cl	1-Methyl-3-octyl-1H-imidazolium chloride	23.19	1.99*	0.50	David et al. (2003)
C4mim-SCN	1-butyl-3-methylimidazolium thiocyanate	24.72	2.13	0.47	Doman´ ska et al. (2009)
C1mim-CH3OC2H4SO4	1,3-dimethylimidazolium methoxyethylsulfate	25.18	4.55	0.22	Doman´ ska et al. (2009)
C1mim-MeSO4	1,3-dimethylimidazolium methylsulfate	28.50	7.69	0.13	Doman´ ska et al. (2009)
C4mim-OcSO4	1-butyl-3-methylimidazolium octylsulfate	24.80	1.43	0.70	Doman´ ska et al. (2009)
C2mim-CF3COO	1-ethyl-3-methylimidazolium trifluoroacetate	25.56	2.75	0.36	Doman´ska et al. (2007)
C8mim-MDEGSO4	1-methyl-3-octylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	23.85	1.39	0.72	Doman´ska et al. (2007)
C6mim-Tf2N	1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	25.23	0.78	miscible	Heintz et al. (2006)
C6mim-Tf2N	1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	25.23	0.75*	miscible	Kato et al. (2005)

Table B2 The mole fraction solubility of ILs in benzene at 298.15 K (Continued)

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	γ_B^{∞}	$x^{exp}{}_B$	Reference
C8mim-Tf2N	1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	24.76	0.63*	miscible	Kato et al. (2005)
C4mPyr-Tf2N	1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide	25.52	0.84*	miscible	Kato et al. (2005)
G6mim-NO3	1-hexyl-3-methylimidazolium nitrate	27.32	1.81	0.55	Supporting Im_Kan (2012)
C1mim-Tf2N	1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	26.42	1.33	0.75	Krummen et al. (2002)
C2mim-Tf2N	1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	26.18	1.18	0.85	Krummen et al. (2002)
C4mim-Tf2N	1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	25.71	0.87	miscible	Krummen et al. (2002)
C2mim-EtSO4	1-ethyl-3-methylimidazolium ethylsulfate	24.45	2.70	0.37	Krummen et al. (2002)
C6mim-BF4	1-hexyl-3-methylimidazolium tetrafluoroborate	31.12	0.96	miscible	Letcher et al. (2003)
C4mPy-BF4	1-butyl-3-methylpyridinium tetrafluoroborate	31.41	1.63	0.61	Letcher et al. (2003)
C2mmim-Tf2N	1-ethyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide	27.46	1.09	0.92	Letcher et al. (2003)
C6mim-PF6	1-hexyl-3-methylimidazolium hexafluorophosphate	28.60	1.05	0.95	Letcher et al. (2003)
C4mim-MDEGSO4	1-butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	24.09	2.04	0.49	Letcher et al. (2005)

Table B2 The mole fraction solubility of ILs in benzene at 298.15 K (Continued)

Ionic Liquid	Ionic Liquid Name	Solubility Parameter^{calc}	γ_B^{∞}	$x^{exp}{}_B$	Reference
C6mim-Tf2N	1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	25.23	0.67	miscible	Letcher et al. (2005)
C2mim-CH3SO3	1-ethyl-3-methylimidazolium trifluoromethanesulfonate	23.14	4.43*	0.23	Doman´ ska (2012)
3C6C14P-PF6	trihexyltetradecylphosphonium hexafluorophosphate	20.50	0.78	miscible	Tumba et al. (2012) extrapolates value
3C6C14P-Tf2N	trihexyltetradecylphosphonium bis (trifluoromethylsulfonyl) imide	17.13	0.37*	miscible	Tumba et al. (2013)
C16mim-BF4	1-hexadecyl-3-methylimidazolium tetrafluoroborate	28.75	0.79	miscible	Mutelet et al. (2007)
C5mPip-NTf2	1-methyl-1-pentylpiperidinium bis(trifluoromethylsulfonyl)imide	22.93	0.70	miscible	Paduszyn´ ski et al. (2013)
C6mPip-NTf2	1-hexyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)imide	22.69	0.67	miscible	Paduszyn´ ski et al. (2013)
C2mim-FAP	1-ethyl-3-methylimidazolium trifluorotris(perfluoroethyl)phosphate	25.18	0.99*	miscible	Zhi-Cheng Tan et al. (2011)
C2mim-TCB	1-ethyl-3-methylimidazolium tetracyanoborate	25.90	1.31*	0.76	Zhi-Cheng Tan et al. (2011)
C6mim-TCB	1-hexyl-3-methylimidazolium tetracyanoborate	24.95	0.73	miscible	Doman´ska et al. (2012)
C10mim-TCB	1-decyl-3-methylimidazolium tetrafluoroborate	24.00	0.58	miscible	Doman´ ska et al. (2010)
C4myr-TCB	1-butyl-3-methylpyridinium tetracyanoborate	25.60	0.81	miscible	Doman´ ska et al. (2011)

Table B2 The mole fraction solubility of ILs in benzene at 298.15 K (Continued)

Ionic Liquid	**Ionic Liquid Name**	**Solubility Parameter^{calc}**	γ_B^{∞}	$x^{exp}{}_B$	**Reference**
NMP	N-Methyl-2-pyrrolidone	23.16	1.04	0.96	Doman´ ska et al. (2012)
Sulfolane	Sulfolane	26.11	2.38	0.42	Doman´ ska et al. (2012)

* extrapolates value

Appendix C Thermodynamic and Physical Properties of Components Considered in PRO/II

The ILs were model as alias component in the Pro/II simulator, using properties as shown in Table C1 (Valderrama and Rojas, 2009). The heats of vaporization for the volatile compounds were predicted with the equation C1 (Hernández, 2013). The parameters for this equation are shown in Table C2 (Hernández, 2013). It should be noticed that due to the non-volatility of the ionic liquid, their enthalpy of vaporization and vapor pressure were set as zero. The VLE diagram of ternary systems containing ILs at different concentration of ILs at T = 300 K and P = 1 atm were calculated using ICAS—utility toolbox to confirm the breaking of the azeotrope. The NRTL (Non Random Two Liquids) thermodynamic model (Renon and Prausnitz, 1968) was used to predict the VLE, the binary interaction parameter and non-random factor were taken from the available literatures (Zhao *et al.*, 2006, Calvar *et al.*, 2008, Hernández, 2013). The liquid enthalpy was estimated by Lee-Kesler (LK) method and the vapor enthalpy was predicted by the Soave-Redlich-Kwong equation of state (SRK).

Table C1 Properties of selected ionic liquids (Valderrama and Rojas, 2009)

Ionic Liquids	Molar mass	ρ_L [g/cm^3]	T_b [K]	T_C [K]	P_C [bar]	V_C [cm^3/mol]	Zc	ω
[C_2mim][$EtSO_4$]	236.3	1.265	712.7	1067.5	40.5	659.8	0.3008	0.3744
[C_1mim][DMP]	222.2	1.2587	590	816.8	27.2	626.8	0.2509	0.5973
[C_2mim][Ac]	170.2	1.0977	578.8	807.1	29.2	544	0.2367	0.5889
[C_2mim][$N(CN)_2$]	177.2	1.1019	737.2	999	29.1	597.8	0.2095	0.7661

$$\Delta H^{vap}\ [kJmol^{-1}] = A\left(1 - \frac{T[K]}{Tc[K]}\right)^{n} \qquad (C1)$$

Table C2 Heat of vaporization parameter for Ethanol, Water, and EG (Hernández, 2013)

Compound	A	Tc/K	n
Ethanol	60.8036	516.3	0.38
Water	54	647.1	0.34
EG	88.2	645	0.397

Table C3 NRTL interaction parameters for the ternary system ethanol + water + EG. Data are taken from Hernández (2013)

i	**Ethanol**	**Ethanol**	**Water**
j	**Water**	**EG**	**EG**
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij}	-55.169	365.3139	769.0499
b_{ji}	670.444	-88.8285	-443.9649
α_{ij}	0.3031	0.4	0.4

Table C4 NRTL interaction parameters for the ternary system ethanol + water + [C_2mim][$EtSO_4$]. Data are taken from Calvar *et al.* (2008)

i	**Ethanol**	**Ethanol**	**Water**
j	**Water**	**[C_2mim][$EtSO_4$]**	**[C_2mim][$EtSO_4$]**
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij}	536.4	-558.976	-210.388
b_{ji}	-372.78	87932.042	-486.606
α_{ij}	−0.404	0.3018	0.996

Table C5 NRTL interaction parameters for the ternary system ethanol + water + [C_1mim][DMP]. Data are taken from Zhao *et al.* (2006)

i	Ethanol	Ethanol	Water
j	Water	[C_1mim][DMP]	[C_1mim][DMP]
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij}	-61.438	1584.3348	609.266
b_{ji}	675.018	-773.013	-4450.577
α_{ij}	0.3008	0.5927	0.4116

Table C6 NRTL interaction parameters for the ternary system ethanol + water + [C_2mim][Ac]. Taken from (Hernández, 2013)

i	Ethanol	Ethanol	Water
j	Water	[C_2mim][Ac]	[C_2mim][Ac]
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij}	-55.1698	-1426.3862	-1505.8078
b_{ji}	670.4442	-965.9411	-1109.3131
α_{ij}	0.3031	0.4	0.4

Table C7 NRTL interaction parameters for the ternary system ethanol + water + [C_2mim][$N(CN)_2$]. Taken from Hernández (2013)

i	Ethanol	Ethanol	Water
j	Water	[C_2mim][$N(CN)_2$]	[C2mim][$N(CN)_2$]
a_{ij}	0.8065	0	0
a_{ji}	0.5143	0	0
b_{ij}	-266.538	350.132	-289.933
b_{ji}	444.888	-415.384	-222.997
α_{ij}	0.4	0.3	0.3

Table C8 NRTL interaction parameters for the ternary system isopropanol + Water + [C_1mim][DMP]. Data are taken from (Wang *et al.*, 2010)

i	Water	Isopropanol	Water
j	Isopropanol	[C_1mim][DMP]	[C_1mim][DMP]
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij}	830.022	26297.200	609.266
b_{ji}	9.320	-1172.105	-1150.578
α_{ij}	0.300	0.106	0.412

Table C9 NRTL interaction parameters for the ternary system isopropanol + Water + [C_2mim][$N(CN)_2$]. Taken from Zhang *et al.* (2007)

i	Water	Isopropanol	Water
j	Isopropanol	[C_2mim][$N(CN)_2$]	[C_2mim][$N(CN)_2$]
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij}	830.022	273.719	-496.981
b_{ji}	9.320	-172.865	109.297
α_{ij}	0.300	0.300	0.300

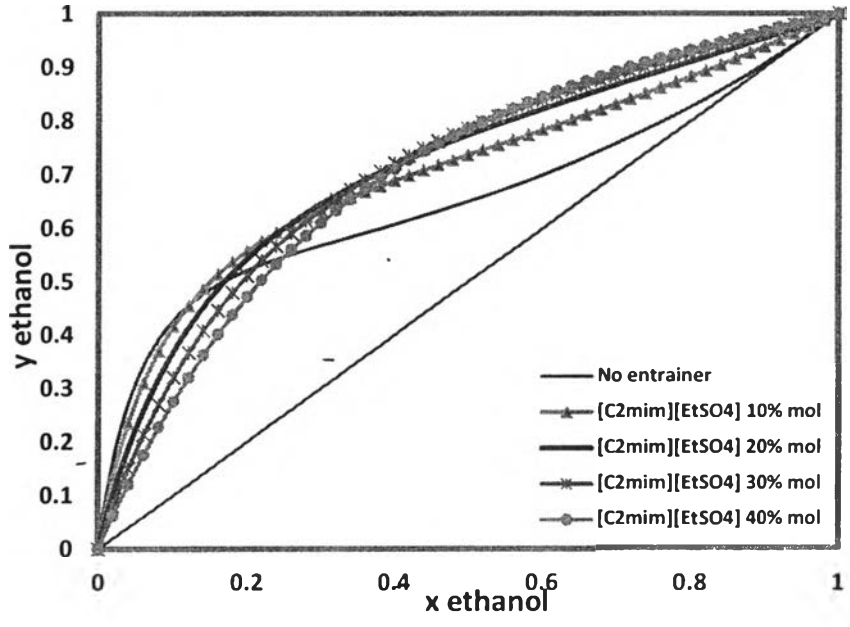

Figure C1 VLE diagram of ethanol + water + $[C_2mim][EtSO_4]$ at different concentration of ILs (using ICAS) at T = 300 K and P = 1 atm.

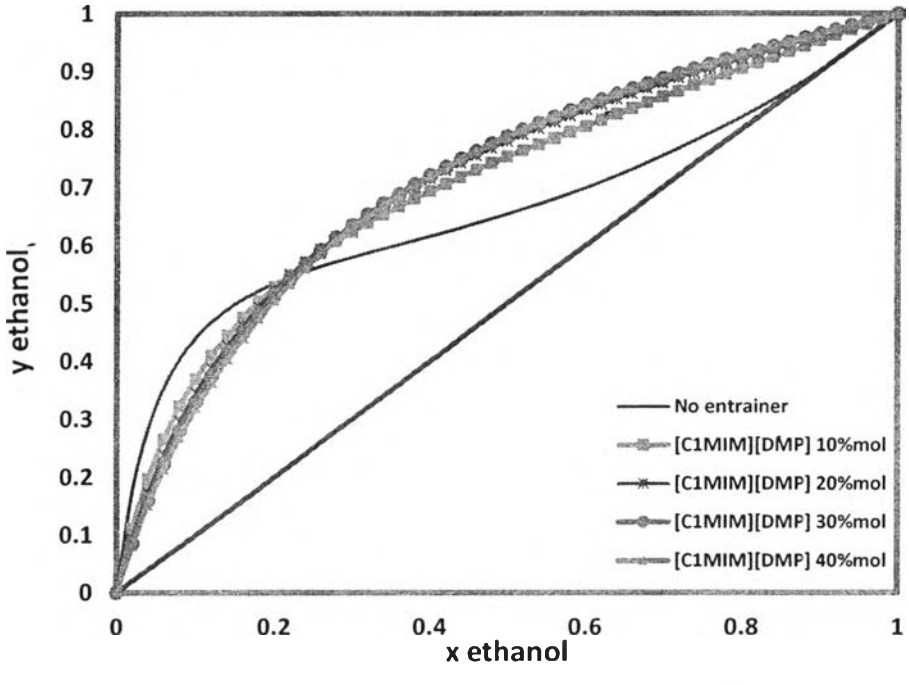

Figure C2 VLE diagram of ethanol + water + $[C_1mim][DMP]$ at different concentration of ILs (using ICAS) at T = 300 K and P = 1 atm.

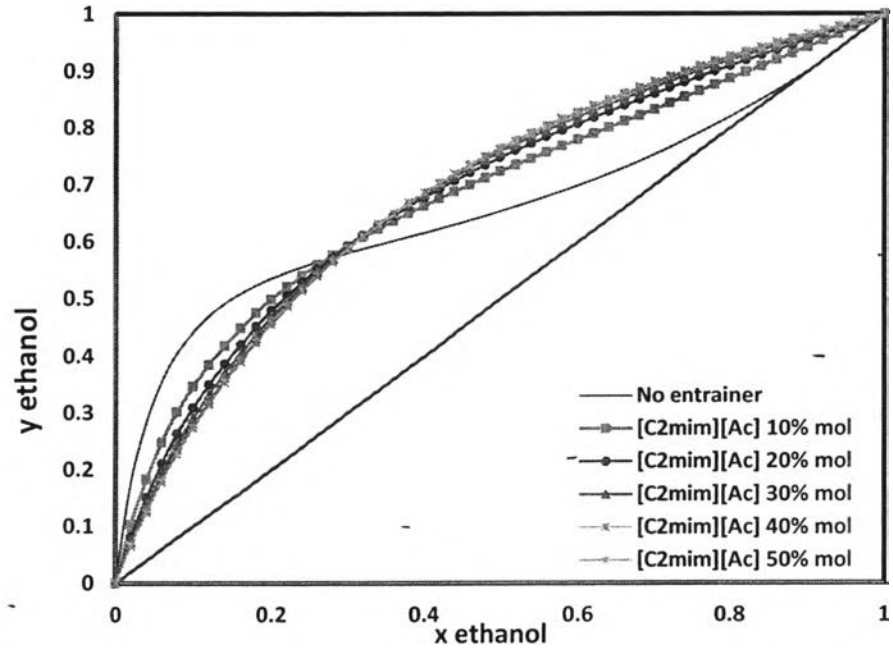

Figure C3 VLE diagram of ethanol + water + $[C_2mim][Ac]$ at different concentration of ILs (using ICAS) at T = 300 K and P = 1 atm.

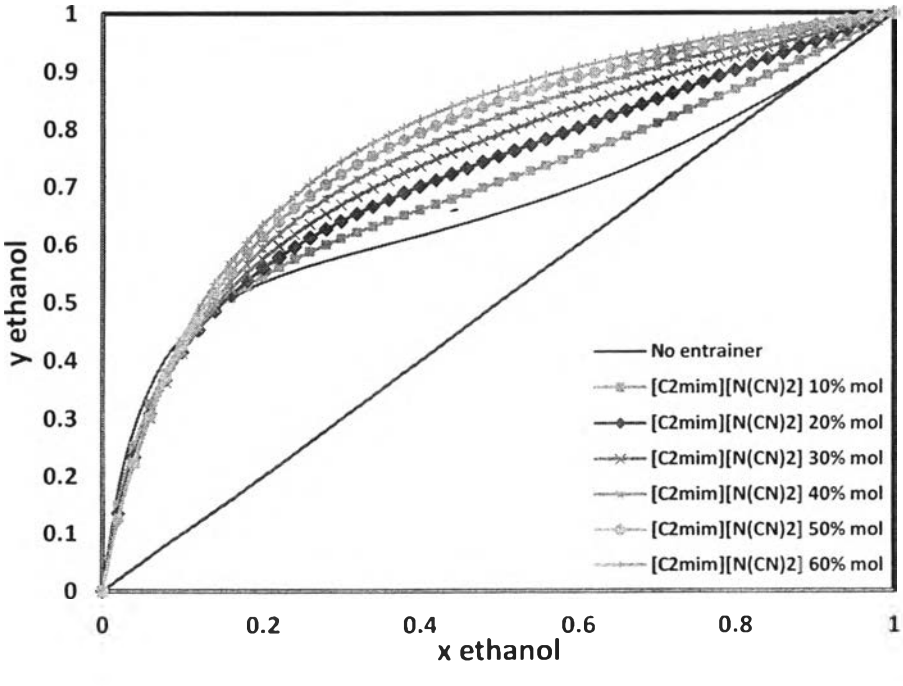

Figure C4 VLE diagram of ethanol + water + $[C_2mim][N(CN)_2]$ at different concentration of ILs (using ICAS) at T = 300 K and P = 1 atm.

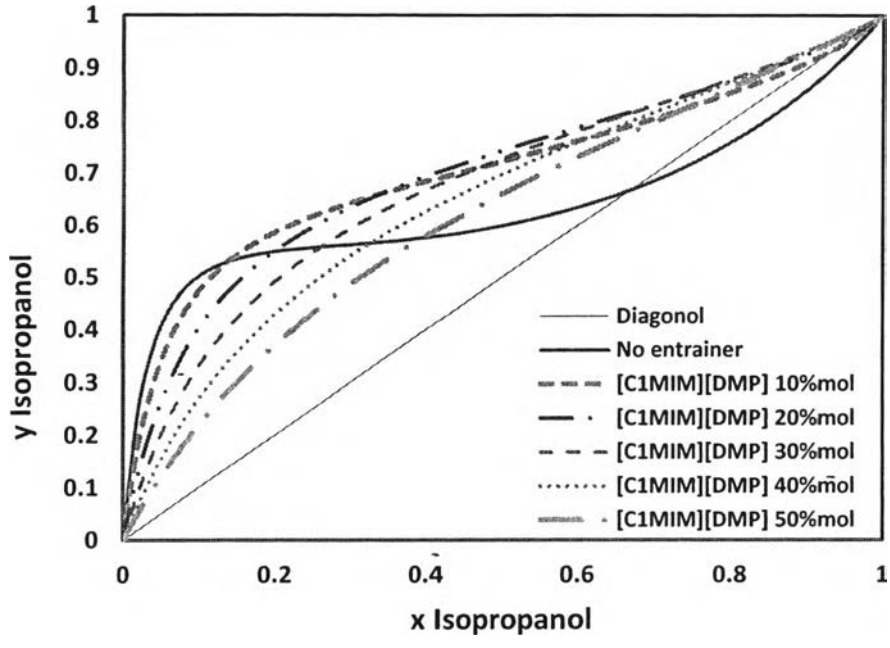

Figure C5 VLE diagram of isopropanol + water + [C_1MIM][DMP] at different concentration of ILs (using ICAS) at T = 300 K and P = 1 atm.

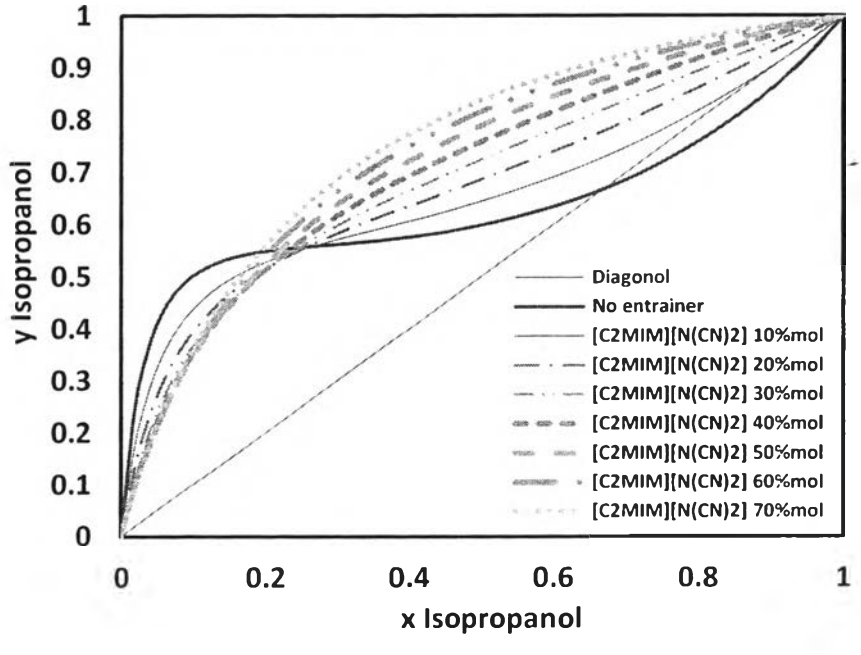

Figure C6 VLE diagram of isopropanol + water + [C_2MIM][$N(CN)_2$] at different concentration of ILs (using ICAS) at T = 300 K and P = 1 atm.

Appendix D Azeotropic Separation Process Flowsheet and Stream Tables Implemented in PRO/II

D.1 Conventional Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using Ethylene Glycol (EG)

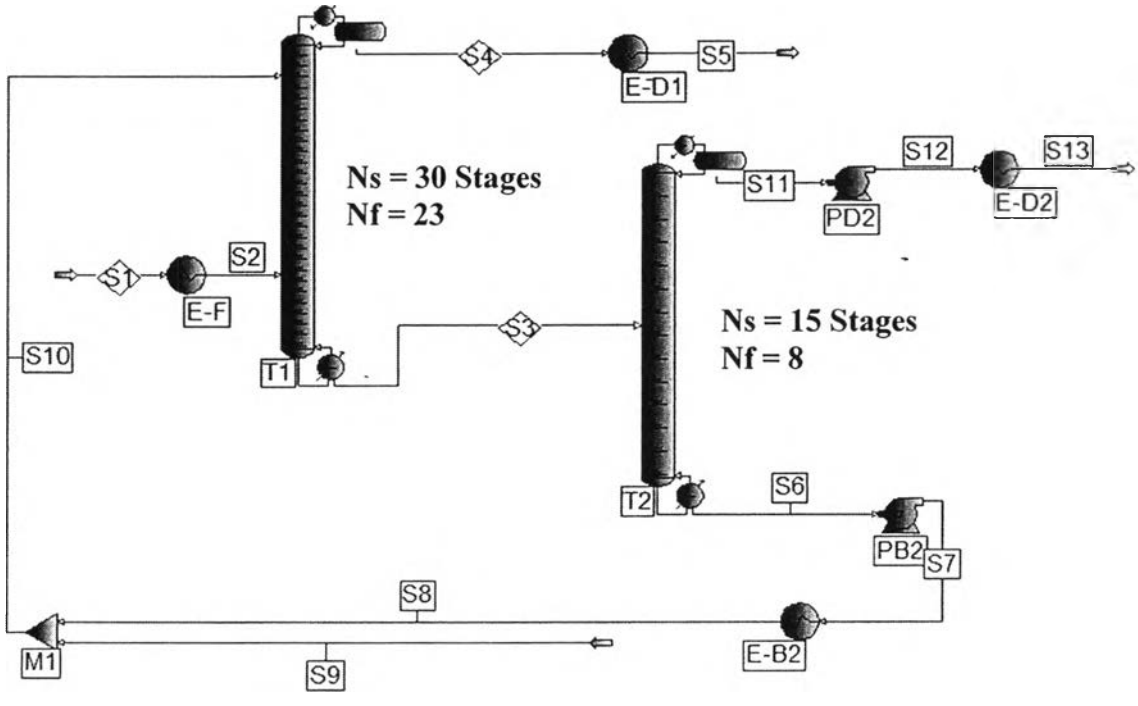

Figure D1 Conventional extractive distillation process flowsheet using ethylene glycol (EG).

Table D1 Extractive distillation column properties using ethylene glycol (EG)

Column Name	Unit	T1	T2
Column Description			
Condenser Duty	MM WATT	-2.9303	-0.8568
Reboiler Duty	MM WATT	3.959	0.681
Column Total Molar Feed	KG-MOL/HR	432.167	272.4458
Column Total Wt. Feed	KG/HR	22489.58	15141.43
Column Condenser Pres	KPA	100	20
Column Condenser Temp	C	77.9697	56.8818
Column Reflux Rate	KG-MOL/HR	112.1374	26.3273
Column Reflux Ratio		0.7021	0.6389

Table D2 Pump properties of the separation process

Pump Name	Unit	PD2	PB2
Pump Description			
Pressure Gain	KPA	80	80
Head	M	8.346	8.0541
Work	KW	0.0182	0.393

Table D3 Heat exchanger properties of the separation process

Hx Name	Unit	E-F	E-D1	E-D2	E-B2
Hx Description					
Duty	MM WATT	0.354	0.307	0.0242	0.8968

Table D4 Stream table of the conventional extractive distillation process using ethylene glycol (EG)

Stream Name	Unit	S1	S4	S3	S11	S6	S10
Stream Description							
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	35.000	77.970	156.167	56.882	150.041	78.000
Pressure	KPA	100.000	100.000	100.000	20.000	20.000	100.000
Total Mass Rate	KG/HR	8091.664	7348.148	15141.433	801.192	14340.242	14400.288
Flowrate	KG-MOL/HR	200.000	159.721	272.446	41.208	231.238	232.205
Total Weight Comp. Rates	KG/HR						
ETHANOL		7371.052	7341.568	29.484	29.484	0.000	0.000
WATER		720.612	6.475	719.171	714.136	5.034	5.034
EG		0.000	0.105	14392.779	57.571	14335.208	14395.254
Total Weight Comp. Fractions							
ETHANOL		0.911	0.999	0.002	0.037	0.000	0.000
WATER		0.089	0.001	0.047	0.891	0.000	0.000
EG		0.000	0.000	0.951	0.072	1.000	1.000
Total Molar Comp. Rates	KG-MOL/HR						
ETHANOL		160.000	159.360	0.640	0.640	0.000	0.000
WATER		40.000	0.359	39.920	39.641	0.279	0.279
EG		0.000	0.002	231.886	0.928	230.958	231.926
Composition							
ETHANOL		0.800	0.998	0.002	0.016	0.000	0.000
WATER		0.200	0.002	0.147	0.962	0.001	0.001
EG		0.000	0.000	0.851	0.023	0.999	0.999

Table D4 Stream table of the conventional extractive distillation process using ethylene glycol (EG) (continue)

Stream Name	Unit	S12	S13	S2	S5	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	56.886	35.000	78.000	35.000	150.059	78.000	78.000
Pressure	KPA	100.000	100.000	100.000	100.000	100.000	100.000	100.000
Total Mass Rate	KG/HR	801.192	801.192	8091.664	7348.148	14340.242	14340.242	60.047
Flowrate	KG-MOL/HR	41.208	41.208	200.000	159.721	231.238	231.238	0.967
Total Weight Comp. Rates	KG/HR							
ETHANOL		29.484	29.484	7371.052	7341.568	0.000	0.000	0.000
WATER		714.136	714.136	720.612	6.475	5.034	5.034	0.000
EG		57.571	57.571	0.000	0.105	14335.208	14335.208	60.047
Total Weight Comp. Fractions								
ETHANOL		0.037	0.037	0.911	0.999	0.000	0.000	0.000
WATER		0.891	0.891	0.089	0.001	0.000	0.000	0.000
EG		0.072	0.072	0.000	0.000	1.000	1.000	1.000
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		0.640	0.640	160.000	159.360	0.000	0.000	0.000
WATER		39.641	39.641	40.000	0.359	0.279	0.279	0.000
EG		0.928	0.928	0.000	0.002	230.958	230.958	0.967
Composition								
ETHANOL		0.016	0.016	0.800	0.998	0.000	0.000	0.000
WATER		0.962	0.962	0.200	0.002	0.001	0.001	0.000
EG		0.023	0.023	0.000	0.000	0.999	0.999	1.000

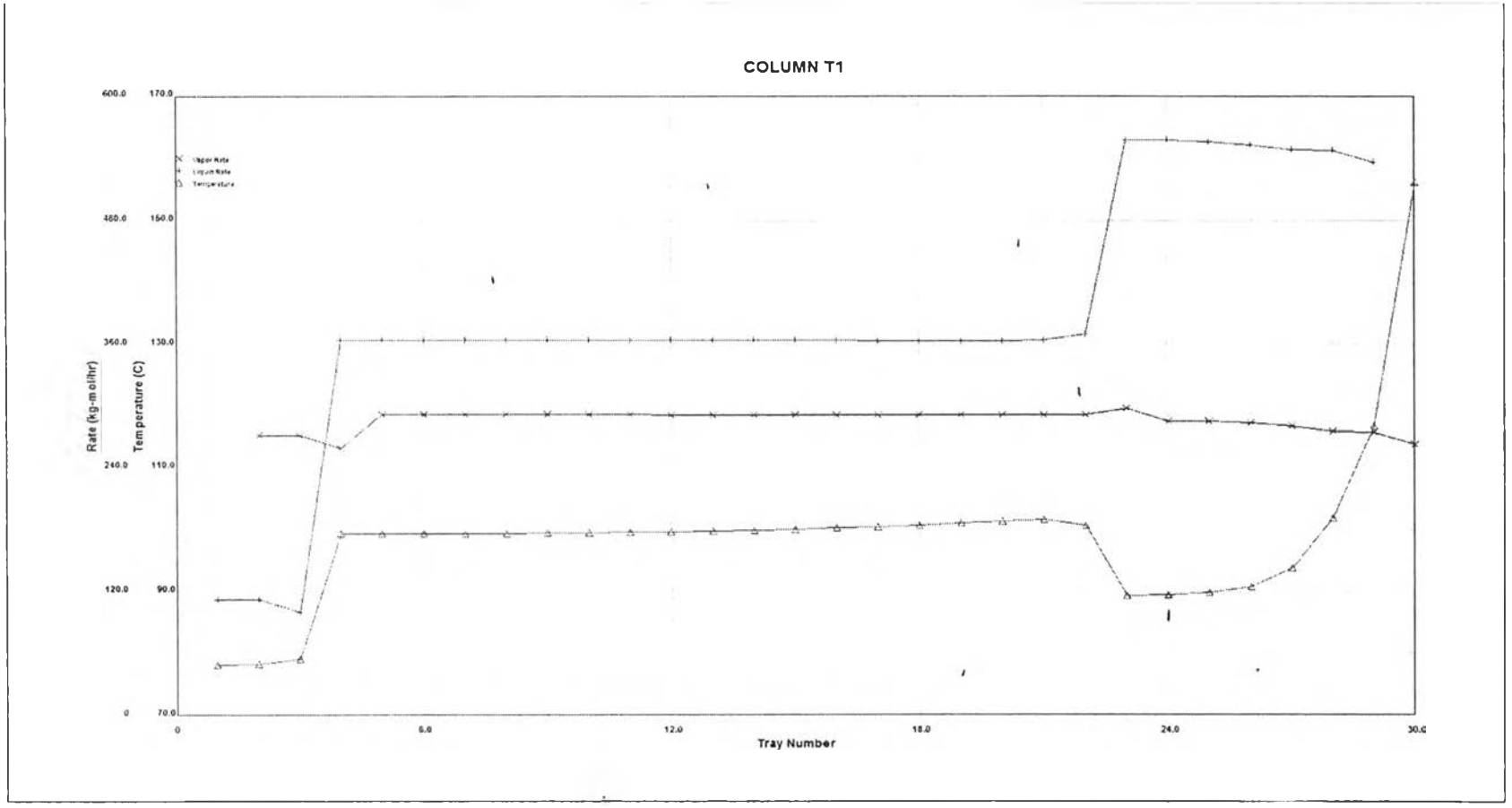

Figure D2 Overview of temperature and flowrate of the extractive distillation process (column T1) using [EG] vs. tray number.

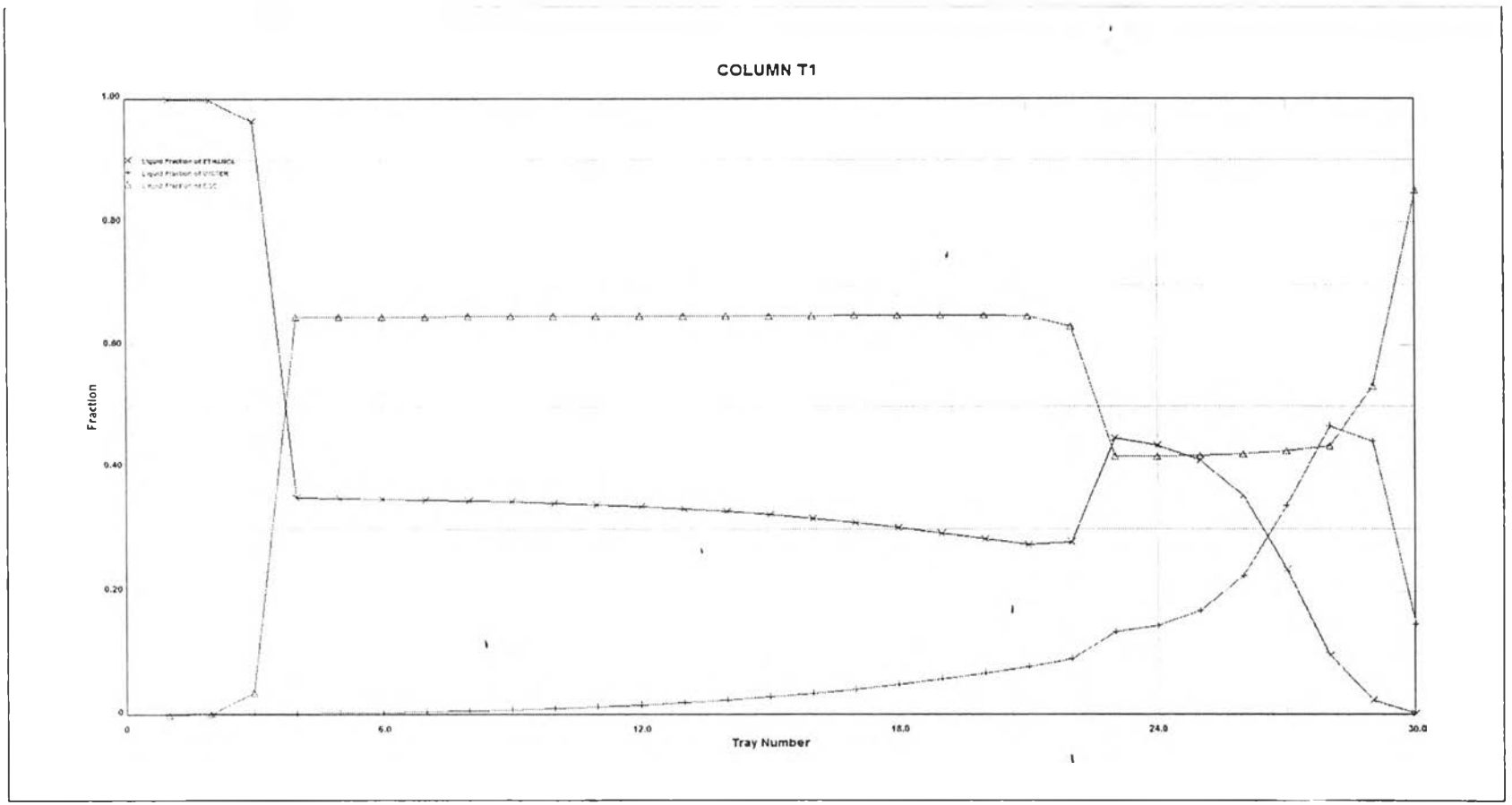

Figure D3 Overview of liquid fraction of the components in the extractive distillation process (column T1) using [EG] vs. tray number.

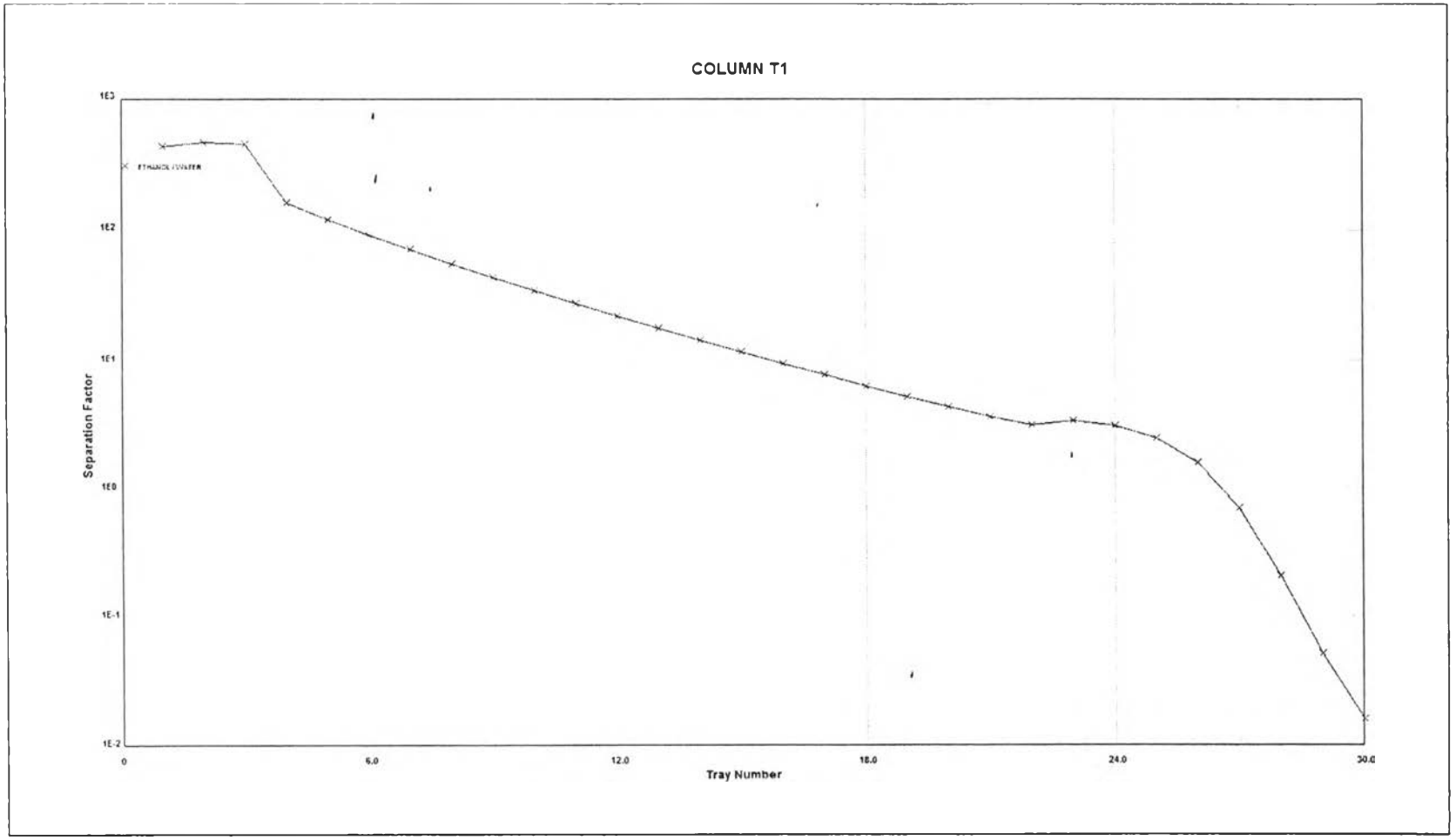

Figure D4 Separation factor in the extractive distillation process (column T1) using [EG] vs. tray number.

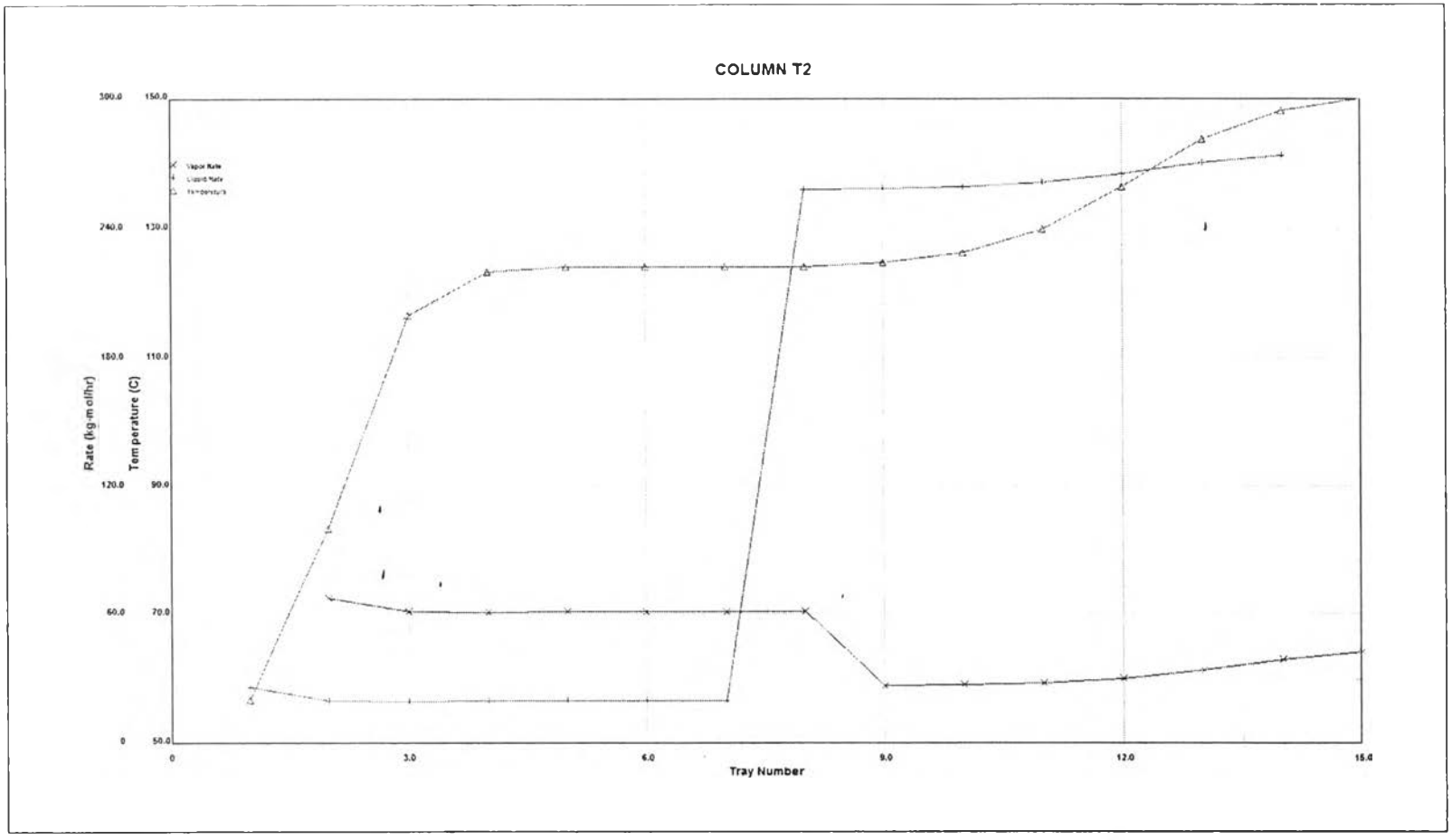

Figure D5 Overview of temperature and flowrate of the recovery process (column T2) using [EG] vs. tray number.

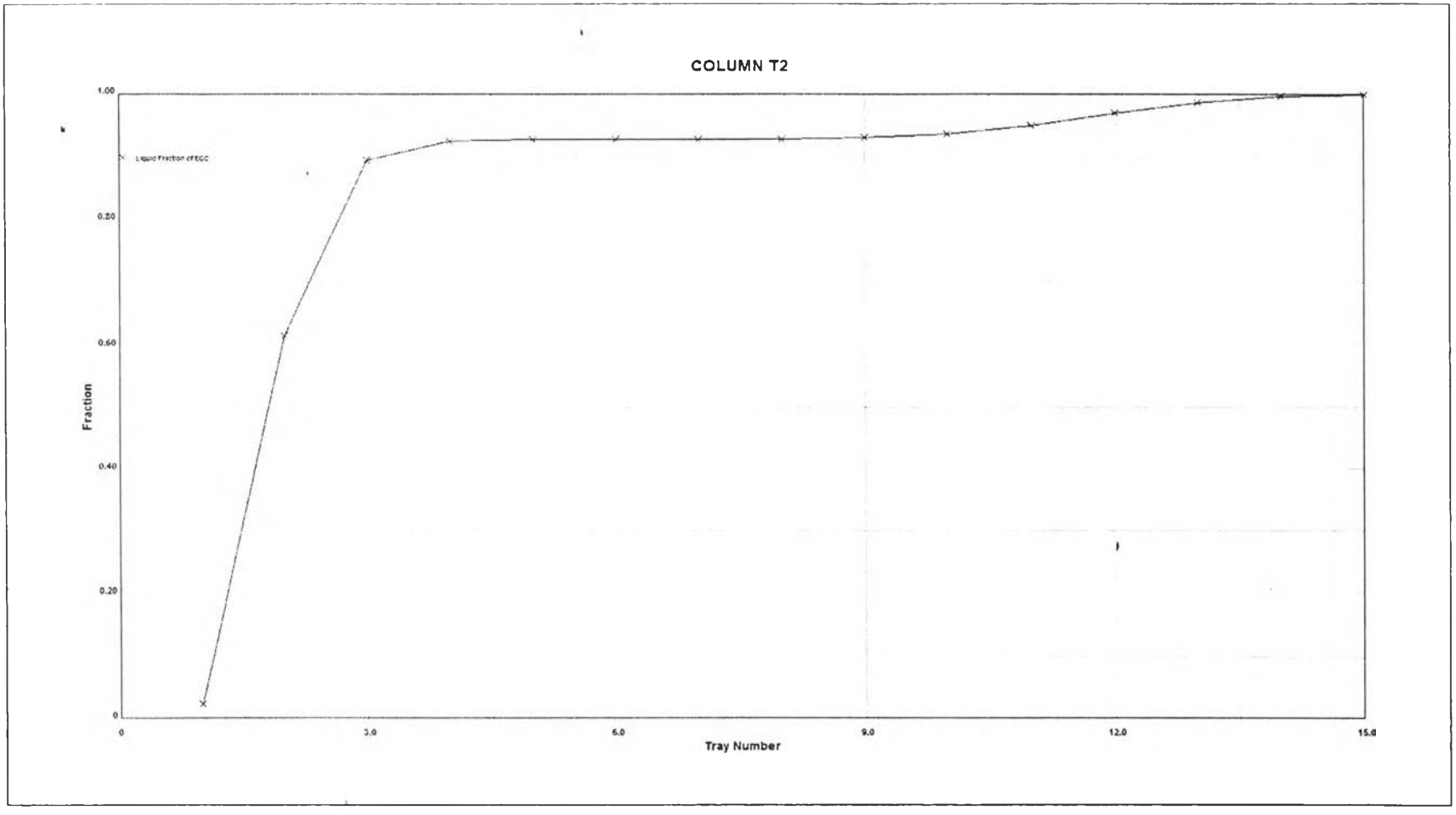

Figure D6 Liquid fraction of EG the recovery process (column T2) using [EG] vs. tray number.

D.2 Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using [C_2mim][$EtSO_4$]

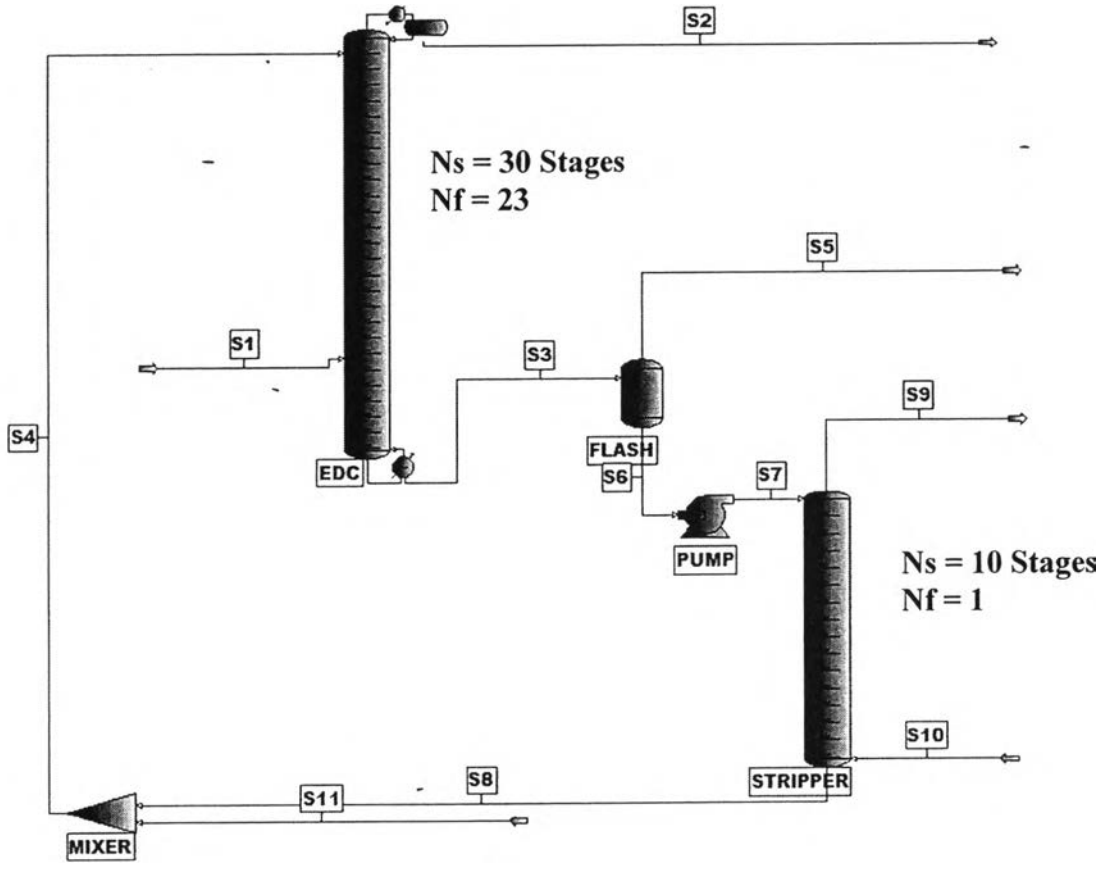

Figure D7 Extractive distillation process flowsheet using [C_2mim][$EtSO_4$].

Table D5 Extractive distillation column properties using $[C_2mim][EtSO_4]$

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.5577
Reboiler Duty	MM WATT	3.4454
Column Total Molar Feed	KG-MOL/HR	285.0747
Column Total Wt. Feed	KG/HR	28179.33
Column Condenser Pres	KPA	100
Column Condenser Temp	C	62.1692
Column Reflux Rate	KG-MOL/HR	136.5369
Column Reflux Ratio		0.8536

Table D6 Flash properties of the separation process using $[C_2mim][EtSO_4]$

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	251
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	0.7529

Table D7 Pump properties of the separation process using $[C_2mim][EtSO_4]$

Pump Name	**Unit**	**P1**
Pump Description		
Pressure Gain	KPA	91.3
Head	M	7.6732
Work	KW	0.4199

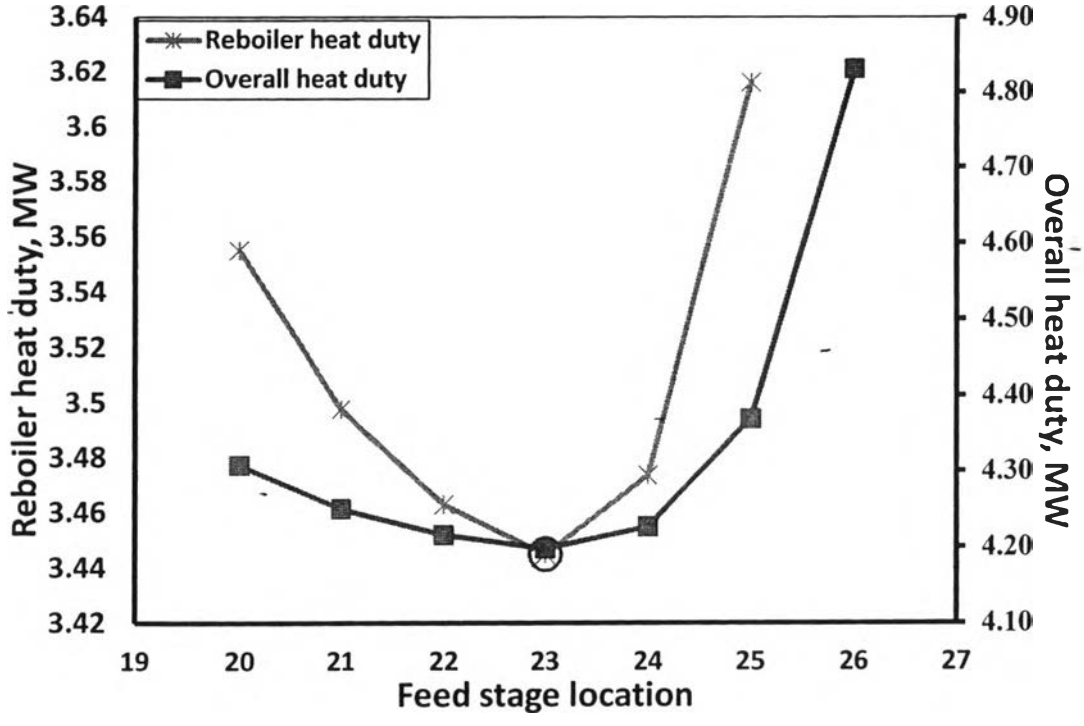

Figure D8 Reboiler heat duty and overall heat duty as a function of feed stage location for separation of the ethanol + water azeotrope using $[C_2mim][EtSO_4]$ = 85.07 kg-mol/hr (fixed Ns = 30 stages).

Table D8 Stream table of the extractive distillation process using $[C_2mim][EtSO_4]$

Stream Name	Unit	S1	S2	S3	S4	S6	S5	S8	S9	S11	S7	S10
Stream Description												
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Vapor	Liquid	Vapor	Liquid	Liquid	Vapor
Temperature	C	78.31	62.17	174.88	78.01	251.00	251.00	78.01	239.63	78.00	251.10	25.00
Pressure	KPA	100.00	100.00	100.00	100.00	10.00	10.00	100.00	100.00	100.00	101.30	100.00
Total Mass Rate	KG/HR	8091.66	7366.56	20812.76	20087.66	20102.79	709.98	20087.66	3813.06	0.00	20102	3797.93
Flowrate	KG-MOL/HR	200.00	159.95	125.12	85.07	85.95	39.17	85.07	132.02	0.00	85.95	131.14
Total Weight Comp. Rates	KG/HR											
ETHANOL		7371.052	7363.686	7.366	0.000	0.184	7.181	0.000	0.184	0.000	0.184	0.000
WATER		720.612	0.719	719.892	0.000	17.098	702.794	0.000	17.098	0.000	17.098	0.000
AIR		0.000	2.159	0.000	2.159	0.000	0.000	2.159	3795	0.000	0.000	3797.933
EMIMESO4		0.000	0.000	20085.503	20085.503	20085.503	0.000	20085.503	0.000	0.000	20085	0.000
Total Weight Comp. Fractions												
ETHANOL		0.911	1.000	0.000	0.000	0.000	0.010	0.000	0.000	0.000	0.000	0.000
WATER		0.089	0.000	0.035	0.000	0.001	0.990	0.000	0.004	0.000	0.001	0.000
AIR		0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.995	0.000	0.000	1.000
EMIMESO4		0.000	0.000	0.965	1.000	0.999	0.000	1.000	0.000	1.000	0.999	0.000
Total Molar Comp. Rates	KG-MOL/HR											
ETHANOL		160	159.840	0.160	0.000	0.004	0.156	0.000	0.004	0.000	0.004	0.000
WATER		40	0.040	39.960	0.000	0.949	39.011	0.000	0.949	0.000	0.949	0.000
AIR		0	0.075	0.000	0.075	0.000	0.000	0.075	131.070	0.000	0.000	131.144
EMIMESO4		0	0.000	85.000	85.000	85.000	0.000	85.000	0.000	0.000	85.000	0.000
Composition												
ETHANOL		0.800	0.999	0.001	0.000	0.000	0.004	0.000	0.000	0.000	0.000	0.000
WATER		0.200	0.000	0.319	0.000	0.011	0.996	0.000	0.007	0.000	0.011	0.000
AIR		0.000	0.000	0.000	0.001	0.000	0.000	0.001	0.993	0.000	0.000	1.000
EMIMESO4		0.000	0.000	0.679	0.999	0.989	0.000	0.999	0.000	1.000	0.989	0.000

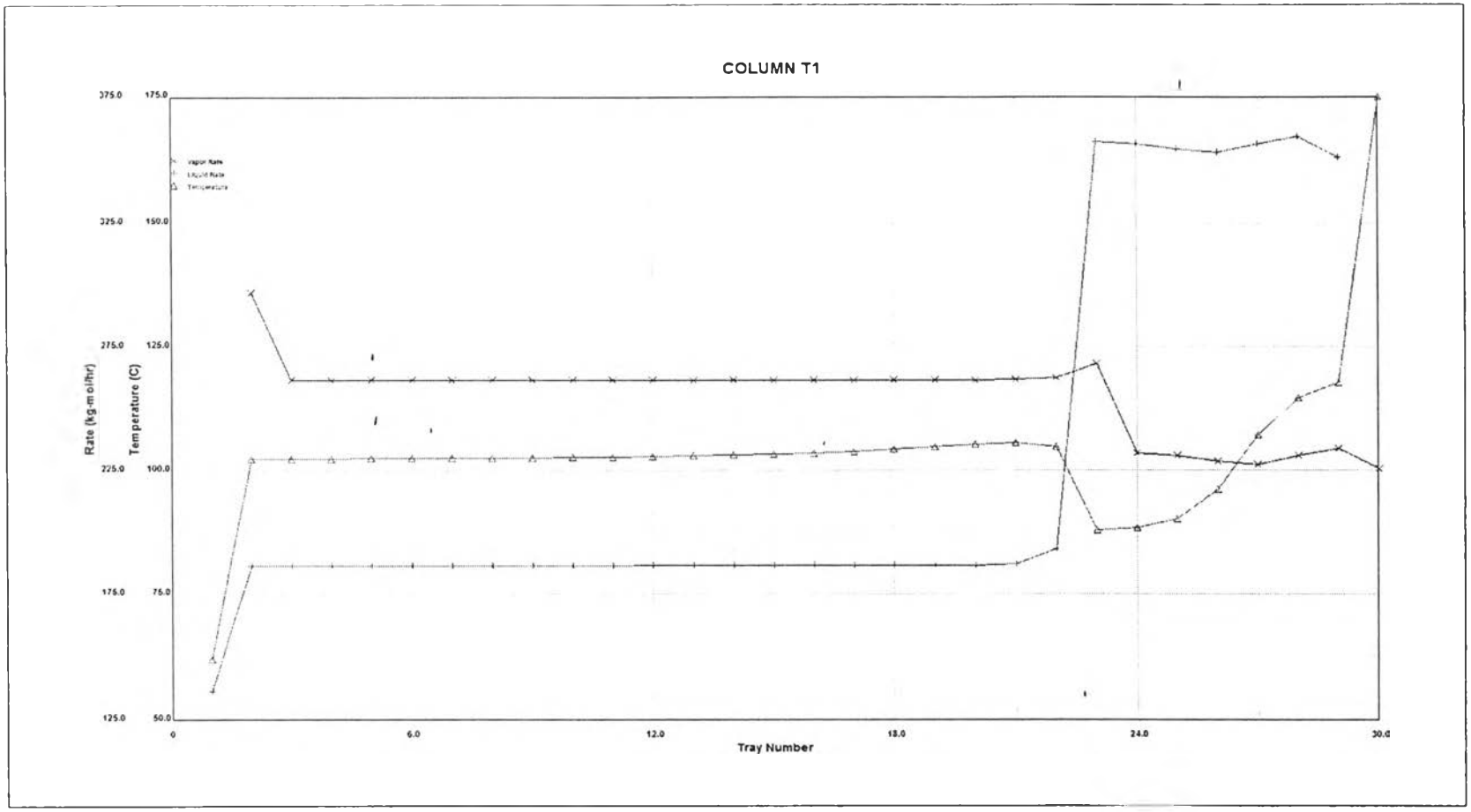

Figure D9 Overview of temperature and flowrate of the extractive distillation process (column T1) using $[C_2mim][EtSO_4]$ vs. tray number.

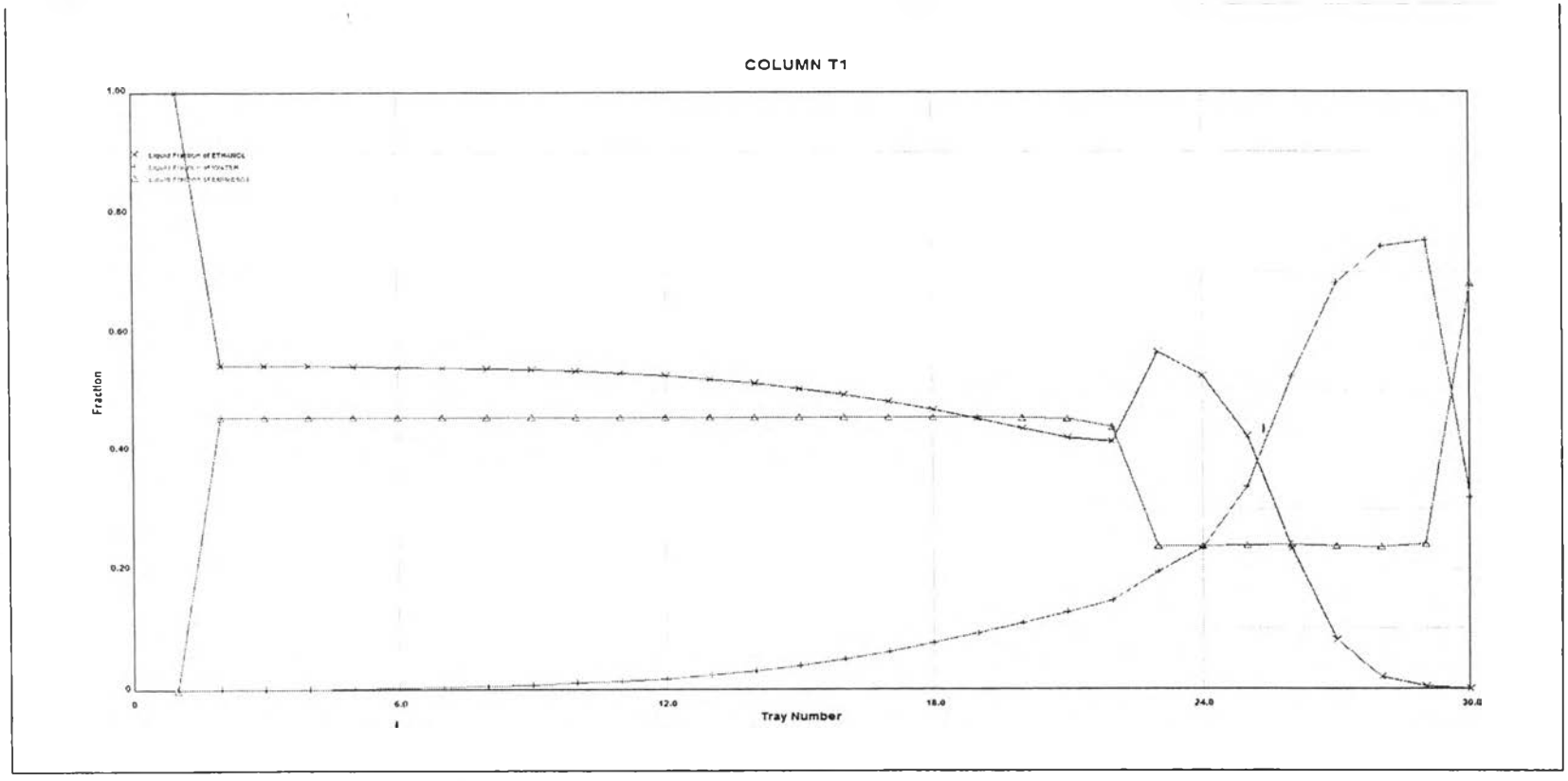

Figure D10 Overview of liquid fraction of the components in the extractive distillation process (column T1) using $[C_2mim][EtSO_4]$ vs. tray number.

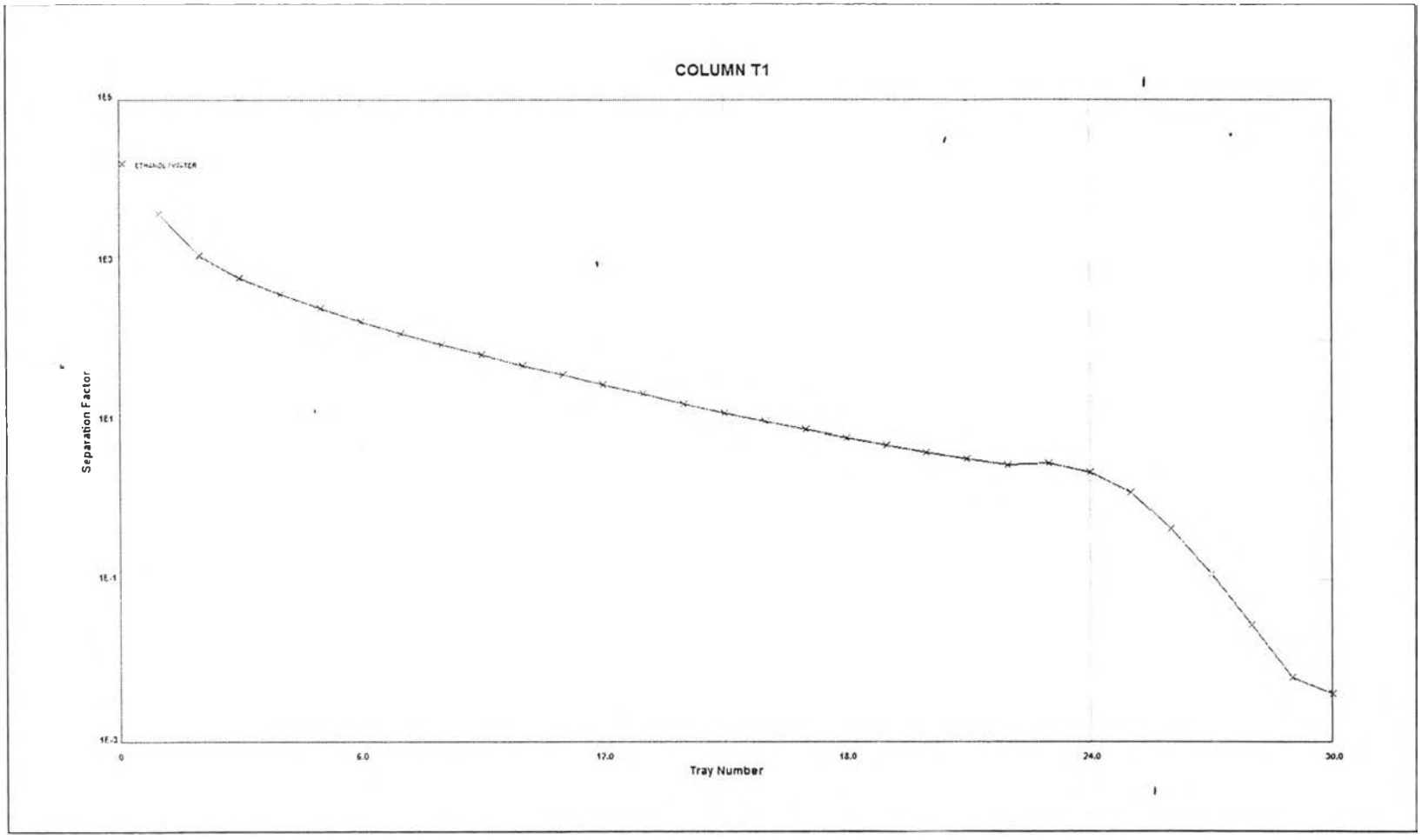

Figure D11 Separation factor in the extractive distillation process (column T1) using $[C_2mim][EtSO_4]$ vs. tray number.

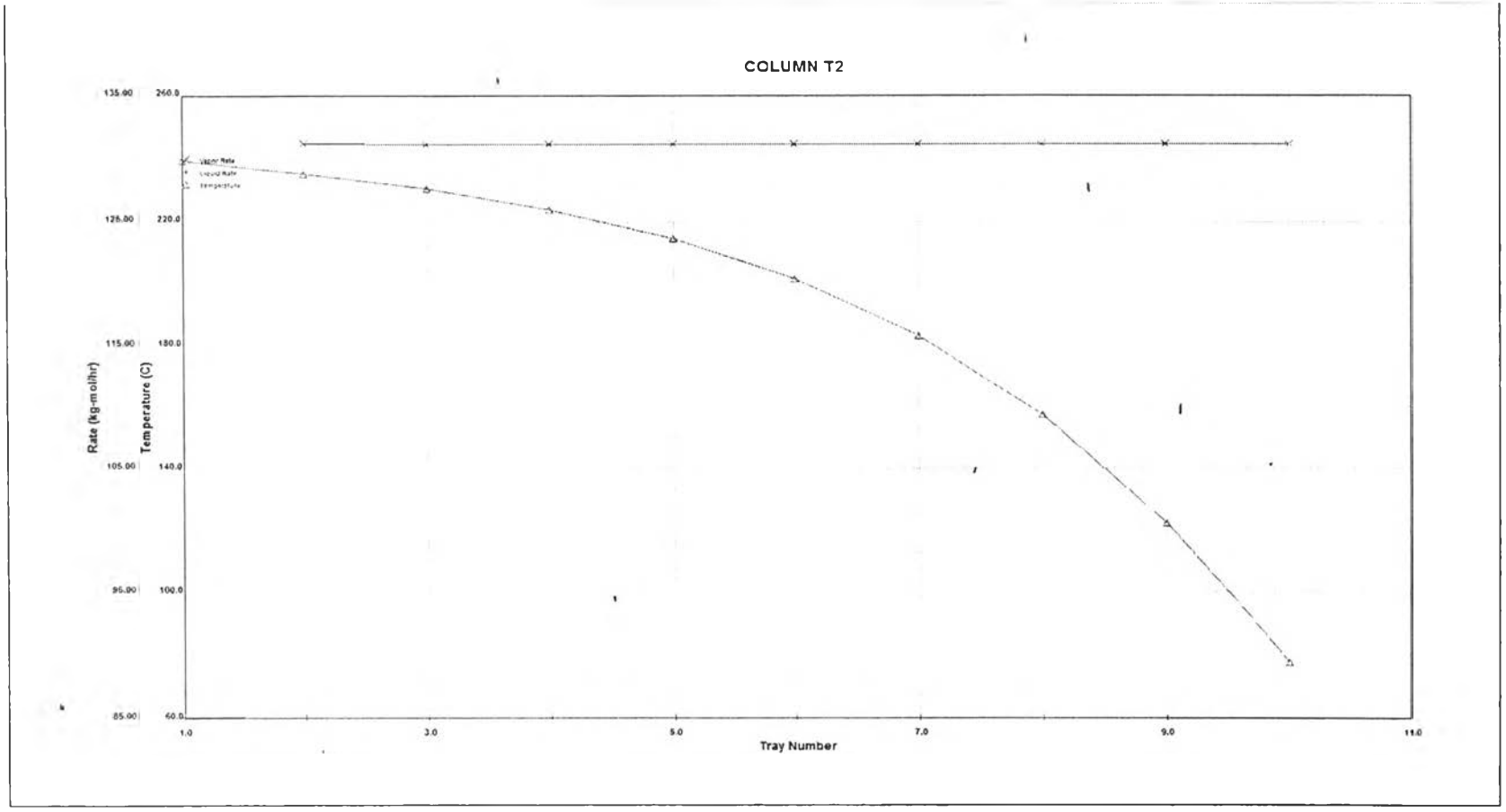

Figure D12 Overview of temperature and flowrate in the stripping column (column T2) using $[C_2mim][EtSO_4]$ vs. tray number.

D.3 Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using [C_1mim][DMP]

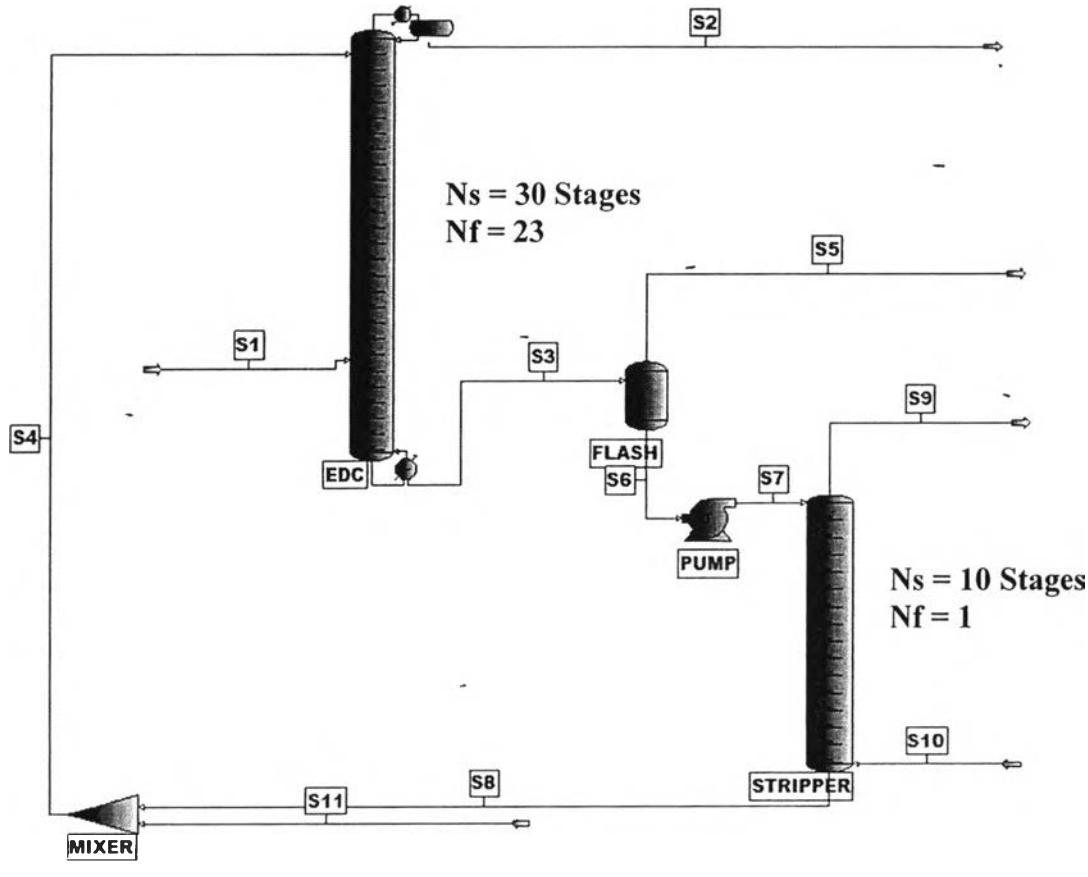

Figure D13 Extractive distillation process flowsheet using [C_1mim][DMP].

Table D9 Extractive distillation column properties using [C_1mim][DMP]

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.0997
Reboiler Duty	MM WATT	3.1641
Column Total Molar Feed	KG-MOL/HR	253.4876
Column Total Wt. Feed	KG/HR	19959.232
Column Condenser Pres	KPA	100
Column Condenser Temp	C	68.6546
Column Reflux Rate	KG-MOL/HR	103.2354
Column Reflux Ratio		0.646

Table D10 Flash properties of the separation process using [C_1mim][DMP]

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	182
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	0.4727

Table D11 Pump properties of the separation process using [C_1mim][DMP]

Pump Name		**P1**
Pump Description		
Pressure Gain	KPA	91.3
Head	M	7.6732
Work	KW	0.4199

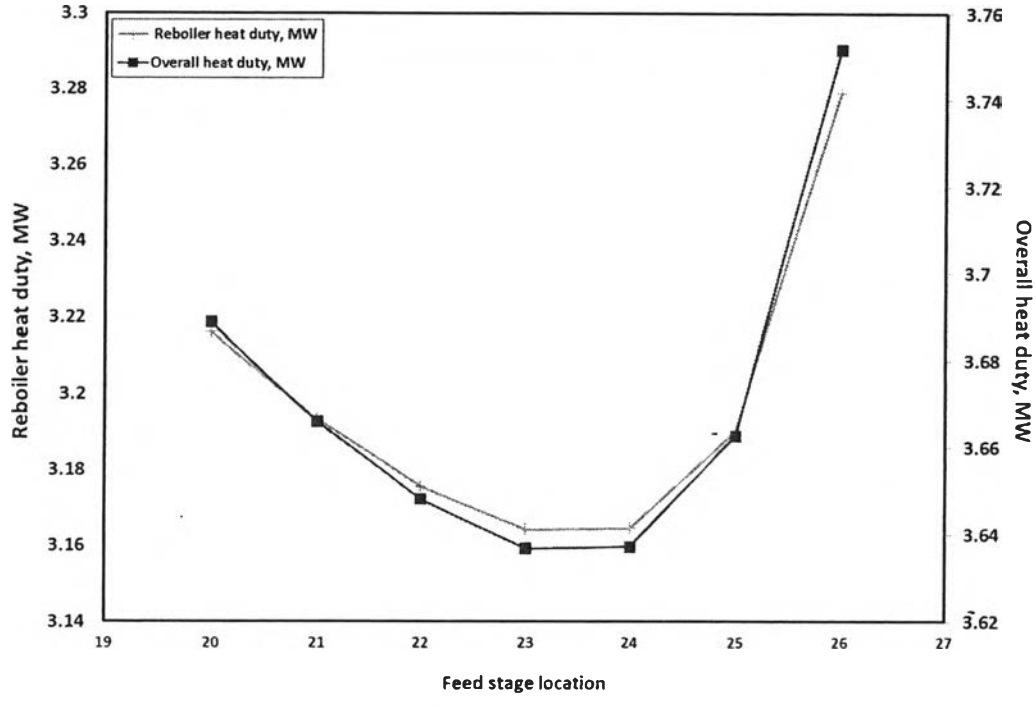

Figure D14 Reboiler heat duty and overall heat duty as a function of feed stage location for separation of the ethanol + water azeotrope using [C_1mim][DMP] = 53.48 kg-mol/hr (fixed Ns = 30 stages).

Table D12 Stream table of the extractive distillation process using [C_1mim][DMP]

Stream Name		S1	S2	S3	S4	S5	S6	S10	S7	S8	S9	S11
Phase		Liquid	Liquid	Liquid	Mixed	Vapor	Liquid	Vapor	Liquid	Liquid	Vapor	Liquid
Temperature	C	78	69	170	78	182	182	25	182	78	165	78
Pressure	KPA	100	100	100	100	10	10	100	100	100	100	100
Total Mass Rate	KG/HR	8091.66	7354.63	12604.60	11867.57	685.83	11918.77	2643.22	11918.77	11867.57	2694.42	n/a
Flowrate	KGMOL/HR	200.000	159.808	93.680	53.487	37.340	56.341	91.271	56.341	53.487	94.124	-0.194
Total Weight Comp. Rates	KG/HR											
ETHANOL		7371.052	7348.939	22.113	0.000	21.594	0.519	0.000	0.519	0.000	0.519	0.000
WATER		720.612	4.335	717.009	0.732	664.237	52.771	0.000	52.771	0.732	52.040	0.000
AIR		0.000	1.357	0.000	1.357	0.000	0.000	2643	0.000	1.357	2641.860	0.000
C1MIMDMP		0.000	0.000	11865.479	11865.479	0.000	11865.479	0.000	11865	11865	0.000	-43.03
Total Weight Comp. Fractions												
ETHANOL		0.911	0.999	0.002	0.000	0.031	0.000	0.000	0.000	0.000	0.000	0.000
WATER		0.089	0.001	0.057	0.000	0.969	0.004	0.000	0.004	0.000	0.019	0.000
AIR		0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.980	0.000
C1MIMDMP		0.000	0.000	0.941	1.000	0.000	0.996	0.000	0.996	1.000	0.000	1.000
Total Molar Comp. Rates	KG-MOL/HR											
ETHANOL		160.000	159.520	0.480	0.000	0.469	0.011	0.000	0.011	0.000	0.011	0.000
WATER		40.000	0.241	39.800	0.041	36.871	2.929	0.000	2.929	0.041	2.889	0.000
AIR		0.000	0.047	0.000	0.047	0.000	0.000	91.271	0.000	0.047	91.224	0.000
C1MIMDMP		0.000	0.000	53.400	53.400	0.000	53.400	0.000	53.400	53.400	0.000	-0.194
Composition												
ETHANOL		0.800	0.998	0.005	0.000	0.013	0.000	0.000	0.000	0.000	0.000	0.000
WATER		0.200	0.002	0.425	0.001	0.987	0.052	0.000	0.052	0.001	0.031	0.000
AIR		0.000	0.000	0.000	0.001	0.000	0.000	1.000	0.000	0.001	0.969	0.000
C1MIMDMP		0.000	0.000	0.570	0.998	0.000	0.948	0.000	0.948	0.998	0.000	1.000

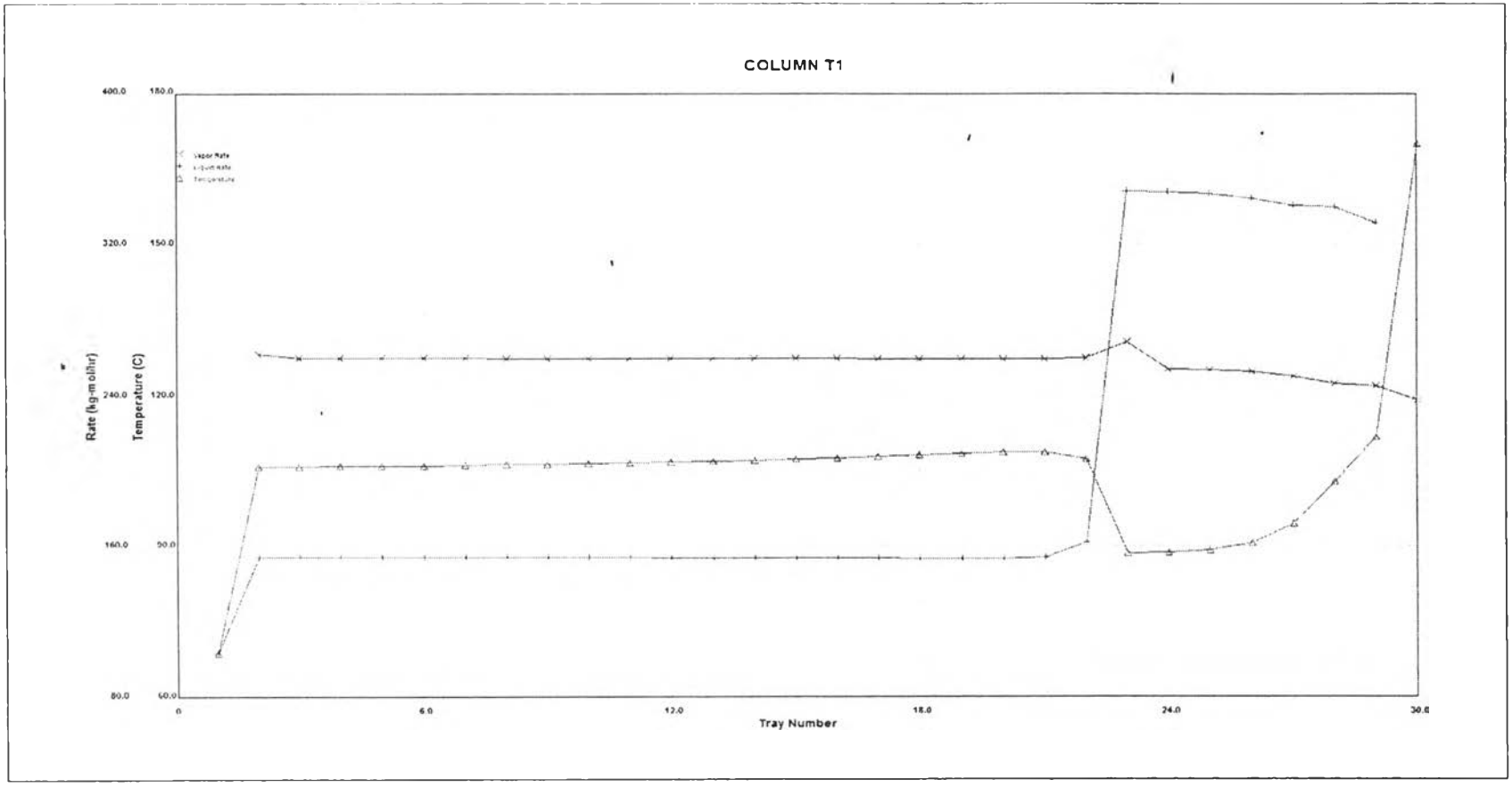

Figure D15 Overview of temperature and flowrate of the extractive distillation process (column T1) using [C_1mim][DMP] vs. tray number.

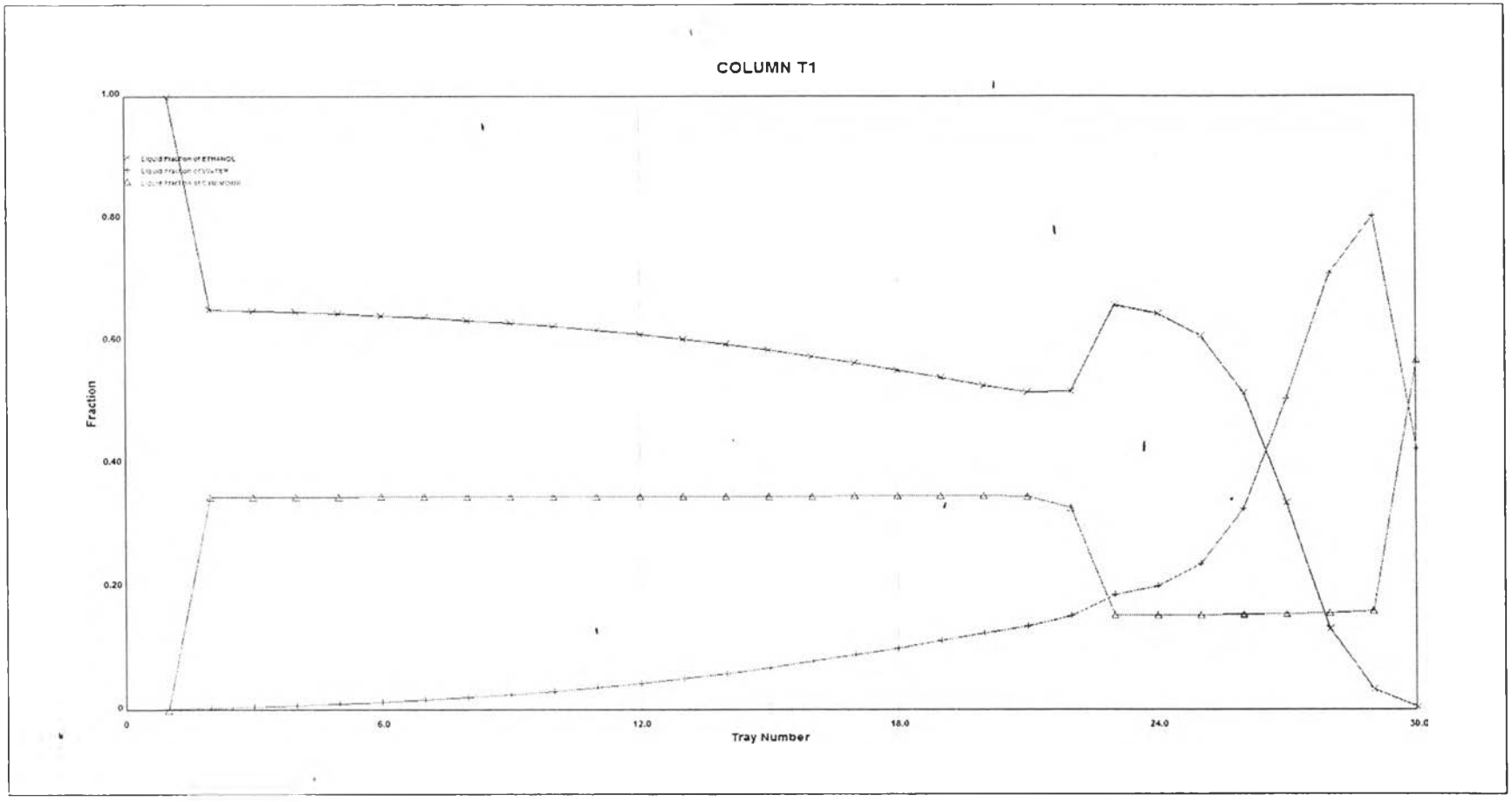

Figure D16 Overview of liquid fraction of the components in the extractive distillation process (column T1) using [C_1mim][DMP] vs. tray number.

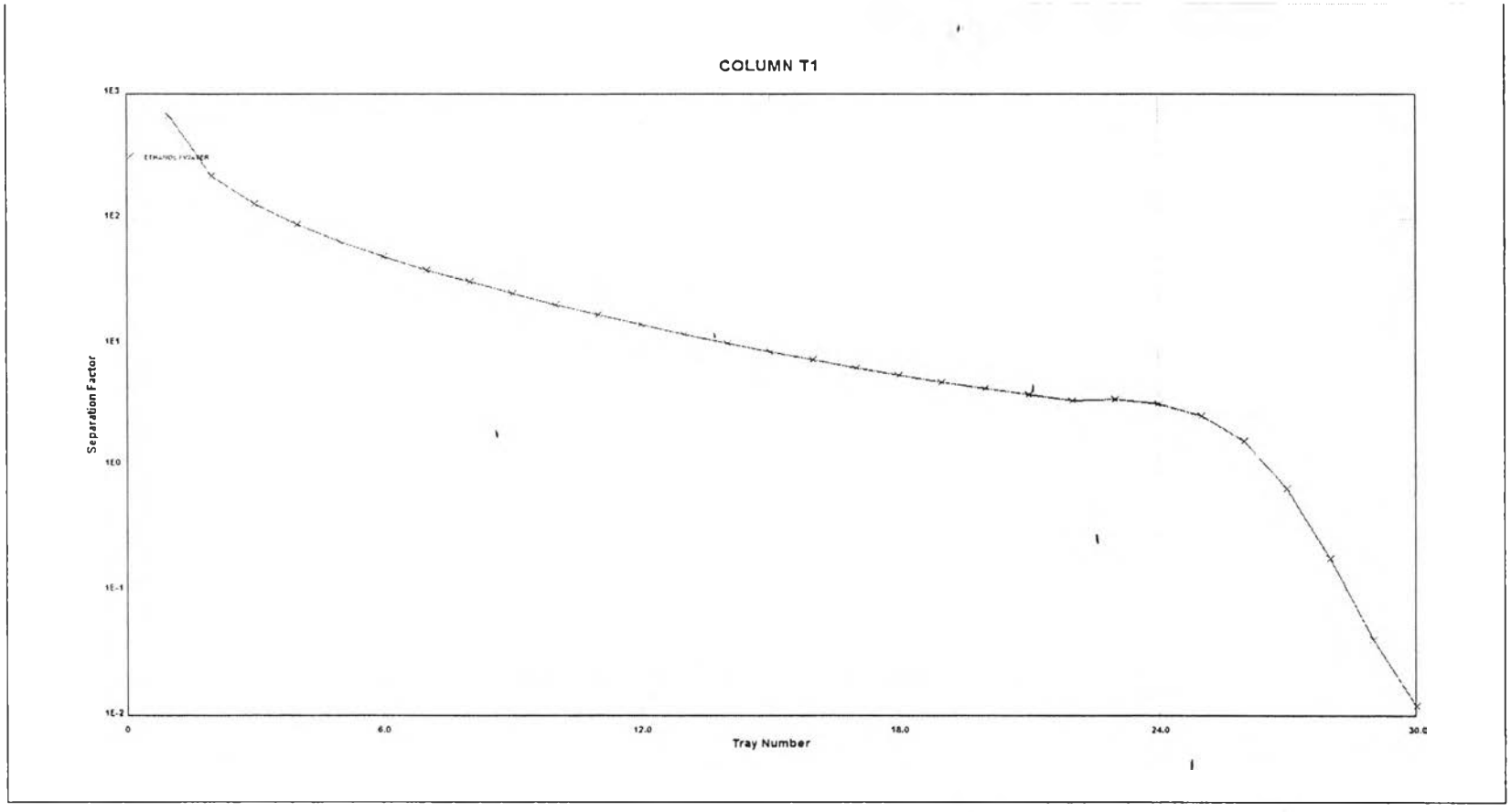

Figure D17 Separation factor in the extractive distillation process (column T1) using $[C_2mim][EtSO_4]$ vs. tray number.

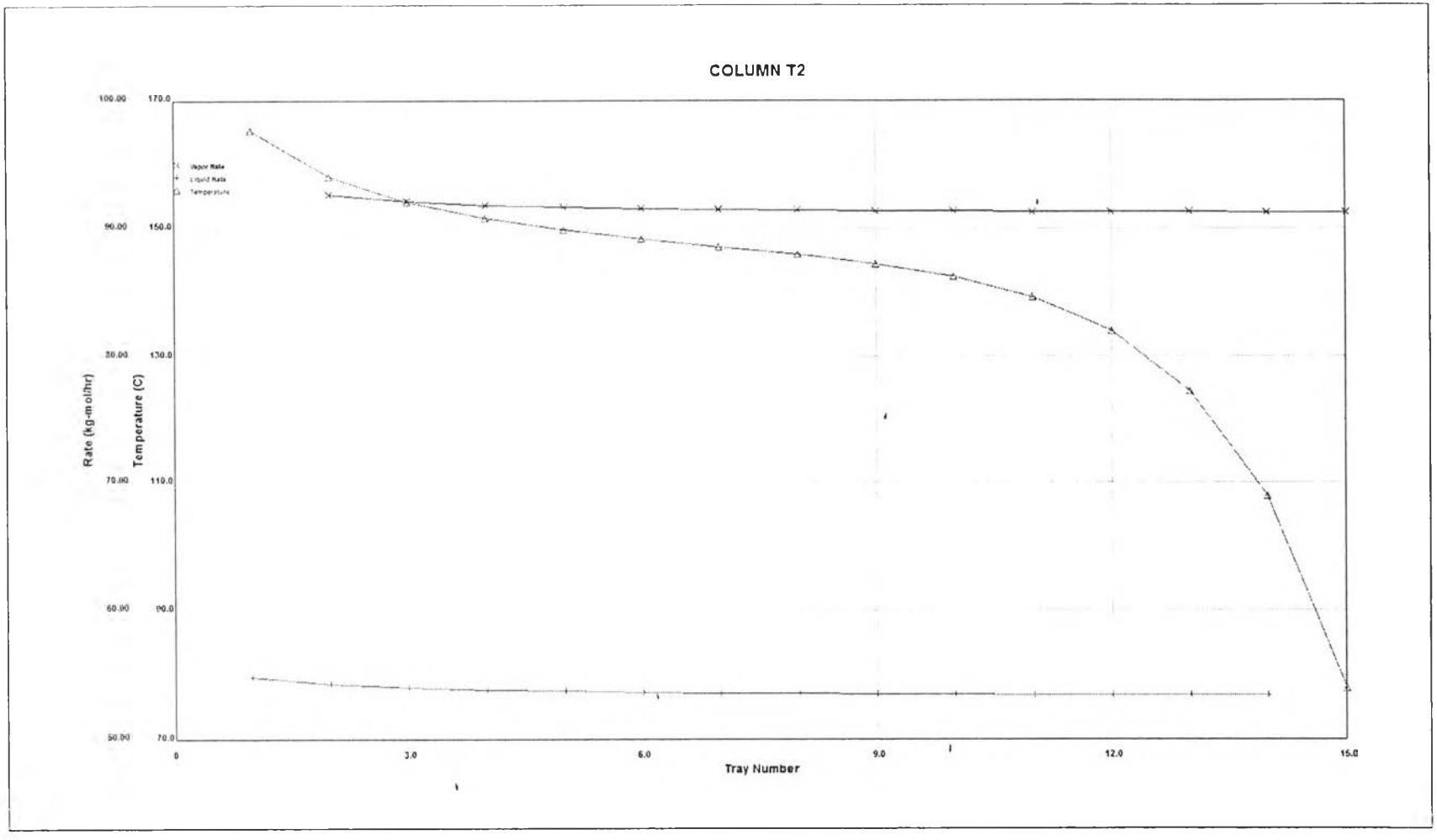

Figure D18 Overview of temperature and flowrate in the stripping column (column T2) using [C_1mim][DMP] vs. tray number.

D.4 Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using [C_2mim][Ac]

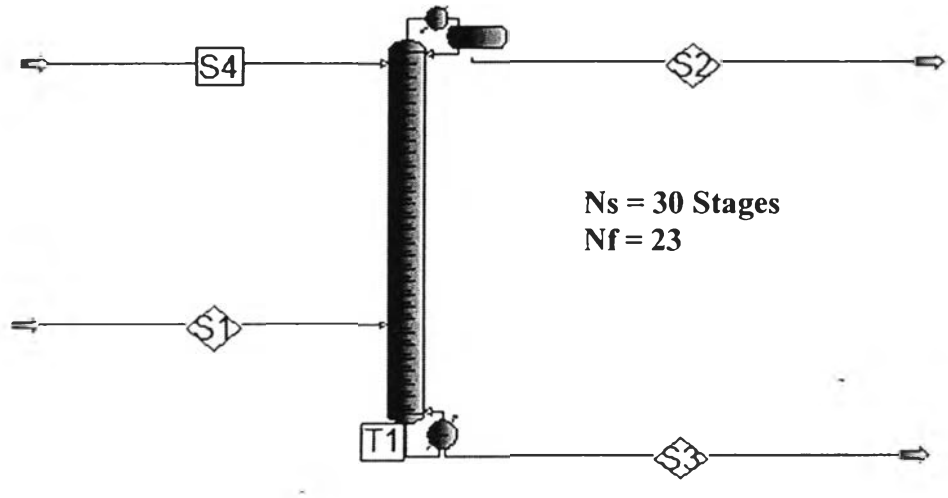

Figure D19 Extractive distillation process flowsheet using [C_2mim][Ac].

Table D13 Extractive distillation column properties using [C_2mim][Ac]

Column Name	Unit	T1
Column Description		
Condenser Duty	MM WATT	-3.9333
Reboiler Duty	MM WATT	3.6211
Column Total Molar Feed	KG-MOL/HR	248.5002
Column Total Wt. Feed	KG/HR	16331.6018
Column Condenser Pres	KPA	25
Column Condenser Temp	C	46.5141
Column Reflux Rate	KG-MOL/HR	158.8303
Column Reflux Ratio		0.9963

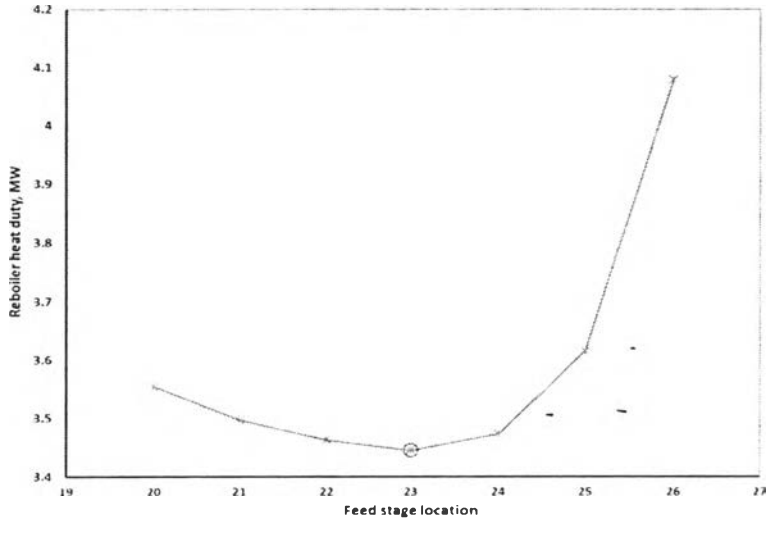

Figure D20 Reboiler heat duty and overall heat duty as a function of feed stage location for separation of the ethanol + water azeotrope using [C_2mim][Ac] = 48.50 kg-mol/hr (fixed Ns = 30 stages).

Table D14 Stream table of the extractive distillation process using [C_2mim][Ac]

Stream Name		S1	S2	S3	S4
Stream Description					
Phase		Liquid	Liquid	Liquid	Liquid
Temperature	C	46.639	46.514	152.361	46.600
Pressure	KPA	25.000	25.000	25.000	25.000
Total Mass Rate	**KG/HR**	**8091**	**7333**	**8997**	**8239**
Flowrate	KG-MOL/HR	200.000	159.417	89.083	48.500
Total Weight Comp. Rates	KG/HR				
ETHANOL		7371.052	7326.796	44.256	0.000
WATER		720.612	6.807	715.552	1.747
AIR		0.000	0.000	0.000	0.000
EMIMAC		0.000	0.000	8238	8238
Total Weight Comp. Fractions					
ETHANOL		0.911	0.999	0.005	0.000
WATER		0.089	0.001	0.080	0.000
AIR		0.000	0.000	0.000	0.000
EMIMAC		0.000	0.000	0.916	1.000
Total Molar Comp. Rates	**KG-MOL/HR**				
ETHANOL		160.000	159.039	0.961	0.000
WATER		40.000	0.378	39.719	0.097
AIR		0.000	0.000	0.000	0.000
EMIMAC		0.000	0.000	48.403	48.403
Composition					
ETHANOL		0.800	0.998	0.011	0.000
WATER		0.200	0.002	0.446	0.002
AIR		0.000	0.000	0.000	0.000
EMIMAC		0.000	0.000	0.543	0.998

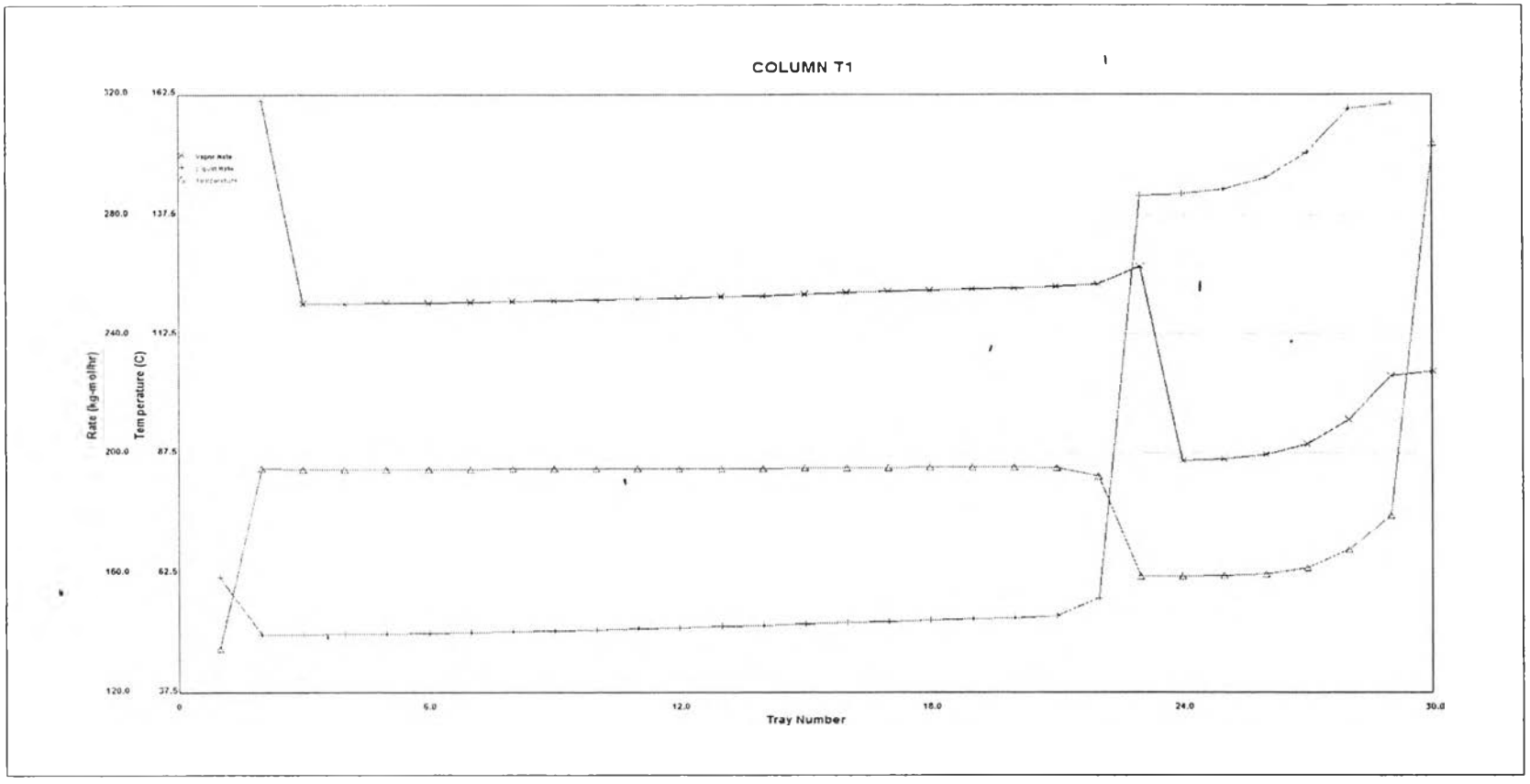

Figure D21 Overview of temperature and flowrate of the extractive distillation process (column T1) using $[C_2mim][Ac]$ vs. tray number.

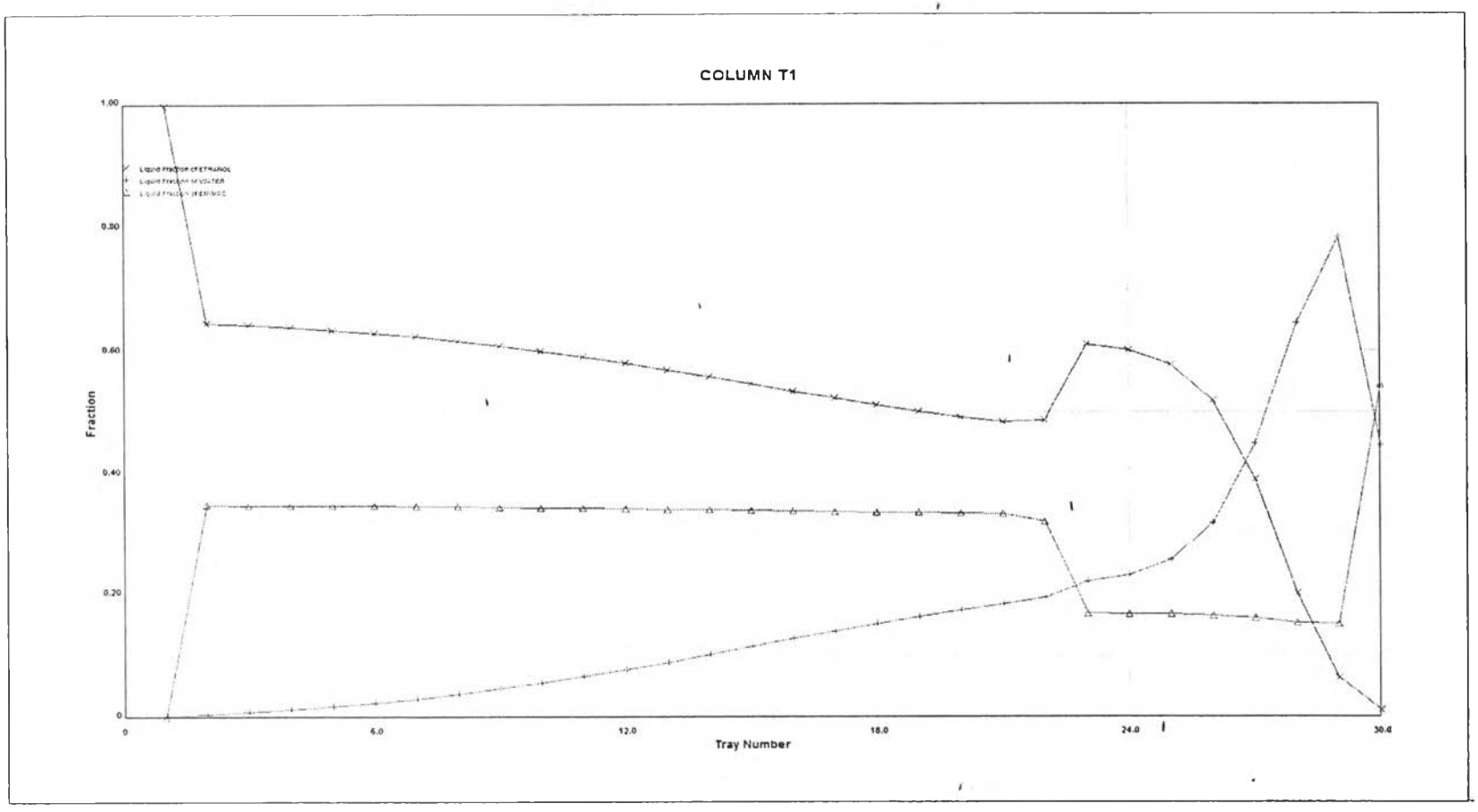

Figure D22 Overview of liquid fraction of the components in the extractive distillation process (column T1) using $[C_2mim][Ac]$ vs. tray number.

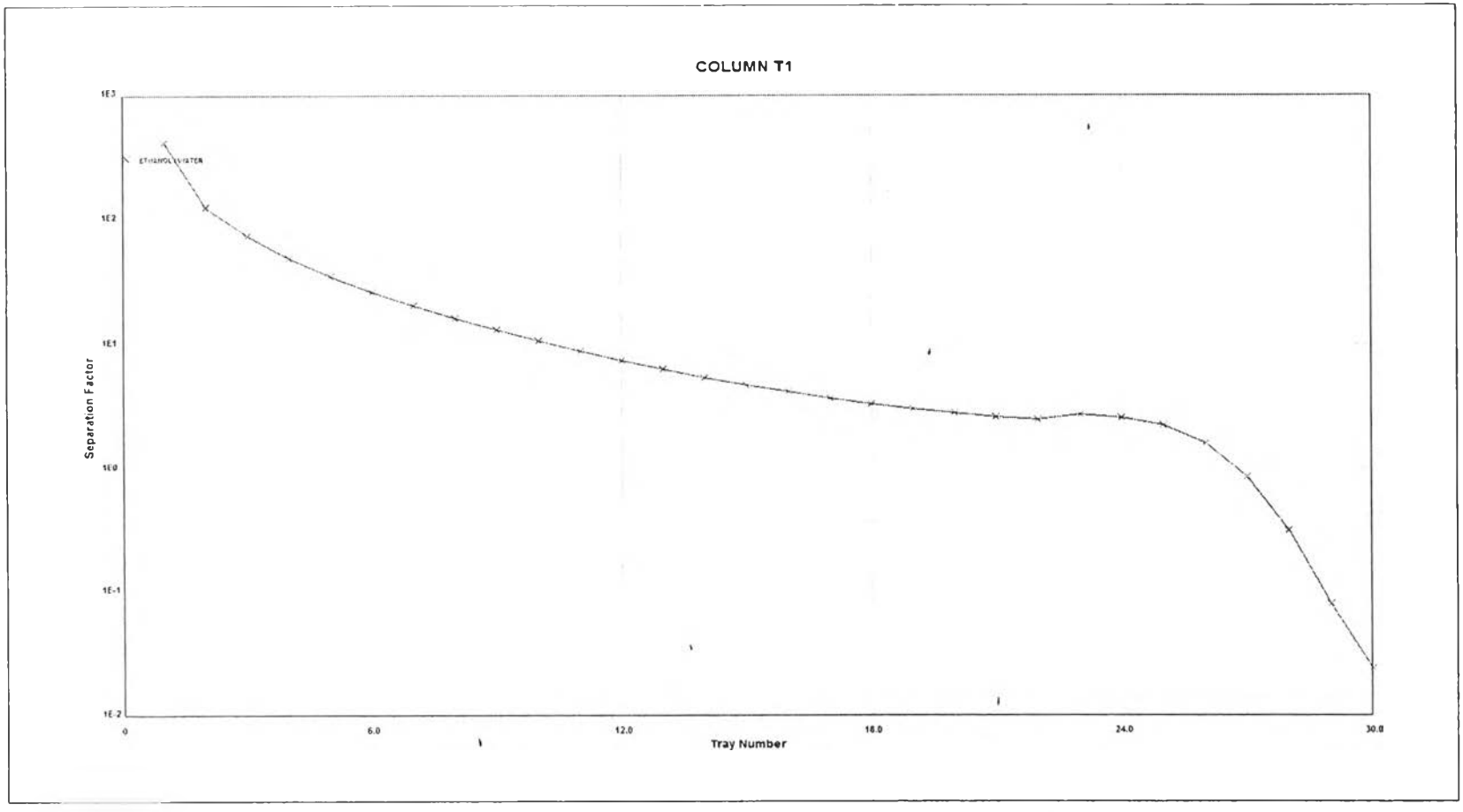

Figure D23 Separation factor in the extractive distillation process (column T1) using [C_2mim][Ac] vs. tray number.

D.5 Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using $[C_2mim][N(CN)_2]$

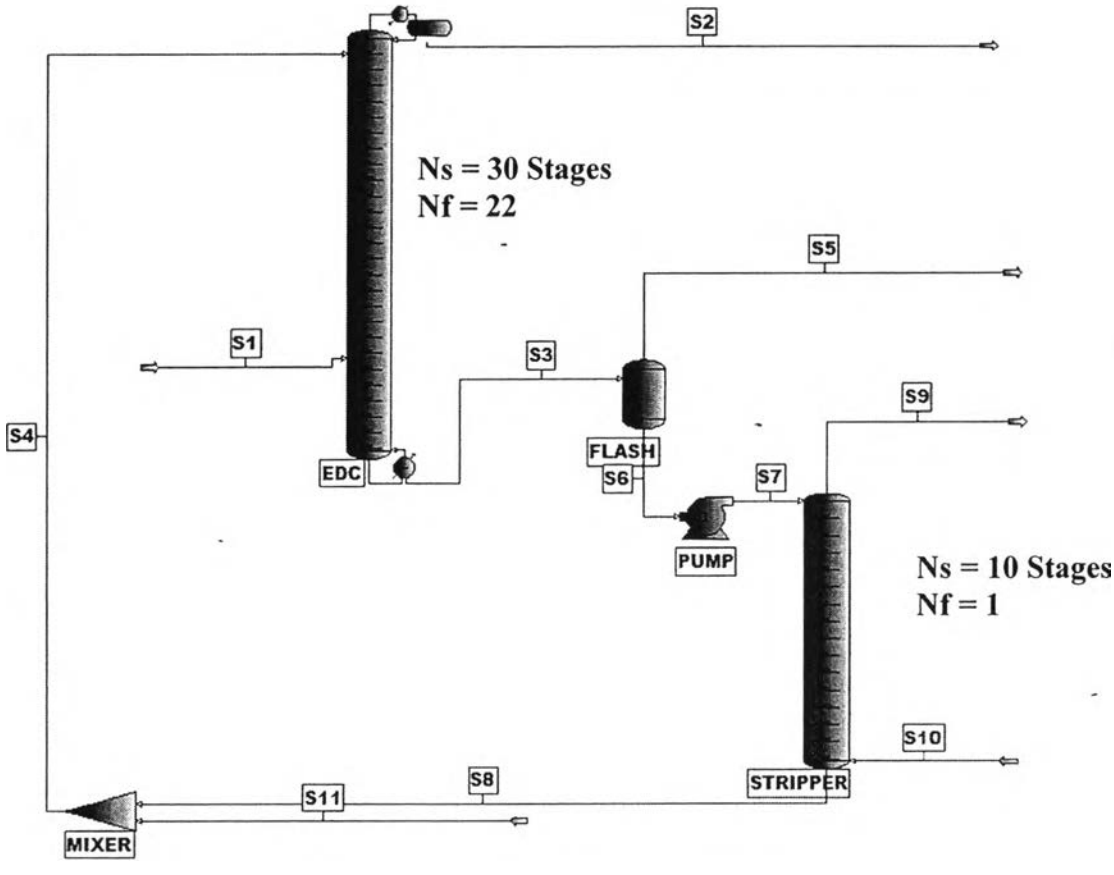

Figure D24 Extractive distillation process flowsheet using $[C_2mim][N(CN)_2]$.

Table D15 Extractive distillation column properties using $[C_2mim][N(CN)_2]$

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.2101
Reboiler Duty	MM WATT	3.3003
Column Total Molar Feed	KG-MOL/HR	319.8652
Column Total Wt. Feed	KG/HR	29316.1726
Column Condenser Pres	KPA	100
Column Condenser Temp	C	53.9168
Column Reflux Rate	KG-MOL/HR	98.0318
Column Reflux Ratio		0.6128

Table D16 Flash properties of the separation process using $[C_2mim][N(CN)_2]$

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	200
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	0.6181

Table D17 Pump properties of the separation process using $[C_2mim][N(CN)_2]$

Pump Name		**P1**
Pump Description		
Pressure Gain	KPA	90
Head	M	8.7377
Work	KW	0.6323

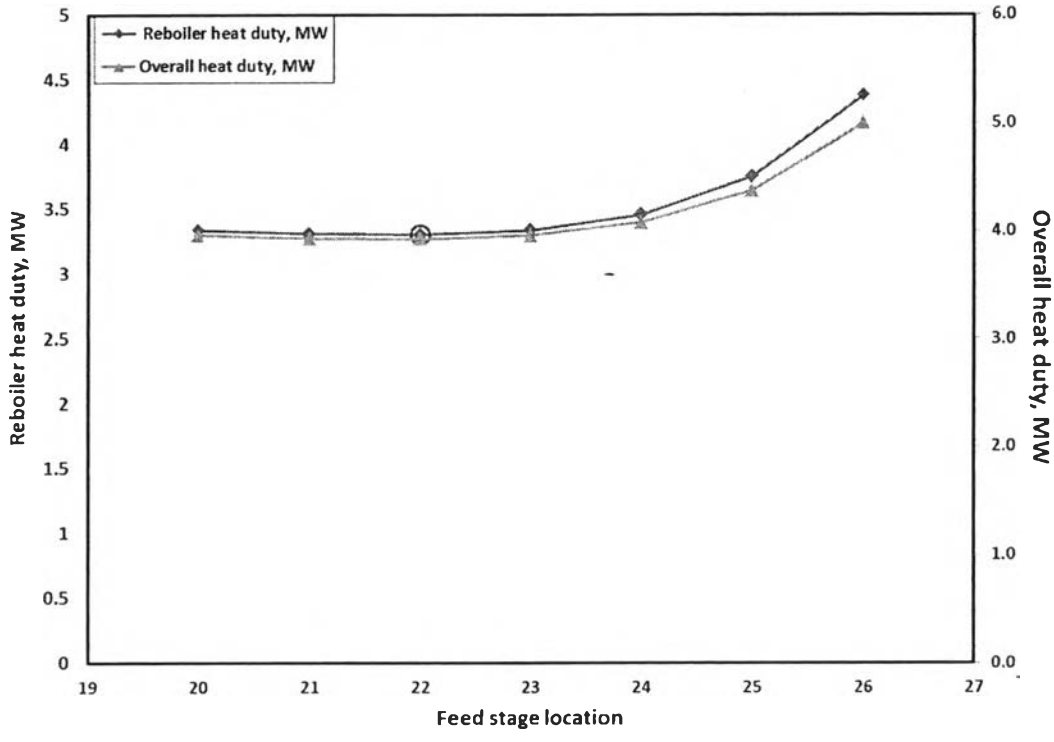

Figure D25 Reboiler heat duty and overall heat duty as a function of feed stage location for separation of the ethanol + water azeotrope using $[C_2mim][N(CN)_2]$= 120 kg-mol/hr (fixed Ns=30 stages).

Table D18 Stream table of the extractive distillation process using $[C_2mim][N(CN)_2]$

Stream Name		S1	S2	S3	S5	S6	S7	S8	S10	S11	S4	S9
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Vapor
Temperature	C	78	54	170	200	200	200	78	25	78	78	191
Pressure	KPA	100	100	100	10	10	100	100	100	100	100	100
Total Mass Rate	KG/HR	8091.6	7367.4	21948.7	682.2	21266.4	21266.4	21224.5	8071.1	n/a	21224.5	8113.0
Flowrate	KG-MOL/HR	200.000	159.985	159.880	37.626	122.254	122.254	119.865	278.698	-0.248	119.865	281.087
Total Weight Comp. Rates	KG/HR											
ETHANOL		7371.052	7363.681	7.371	7.268	0.103	0.103	0.000	0.000	0.000	0.000	0.103
WATER		720.612	0.721	719.891	674.998	44.893	44.893	0.000	0.000	0.000	0.000	44.893
AIR		0.000	3.041	0.000	0.000	0.000	0.000	3.041	8071.1	0.000	3.041	8068.0
EMIMNCN2		0.000	0.000	21221	0.000	21221	21221	21221	0.000	-44	21221	0.000
Total Weight Comp. Fractions												
ETHANOL		0.911	0.999	0.000	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000
WATER		0.089	0.000	0.033	0.989	0.002	0.002	0.000	0.000	0.000	0.000	0.006
AIR		0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.994
EMIMNCN2		0.000	0.000	0.967	0.000	0.998	0.998	1.000	0.000	1.000	1.000	0.000
Total Molar Comp. Rates	KG-MOL/HR											
ETHANOL		160.000	159.840	0.160	0.158	0.002	0.002	0.000	0.000	0.000	0.000	0.002
WATER		40.000	0.040	39.960	37.468	2.492	2.492	0.000	0.000	0.000	0.000	2.492
AIR		0.000	0.105	0.000	0.000	0.000	0.000	0.105	278.698	0.000	0.105	278.593
EMIMNCN2		0.000	0.000	119.760	0.000	119.760	119.760	119.760	0.000	-0.248	119.760	0.000
Composition												
ETHANOL		0.800	0.999	0.001	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000
WATER		0.200	0.000	0.250	0.996	0.020	0.020	0.000	0.000	0.000	0.000	0.009
AIR		0.000	0.001	0.000	0.000	0.000	0.000	0.001	1.000	0.000	0.001	0.991
EMIMNCN2		0.000	0.000	0.749	0.000	0.980	0.980	0.999	0.000	1.000	0.999	0.000

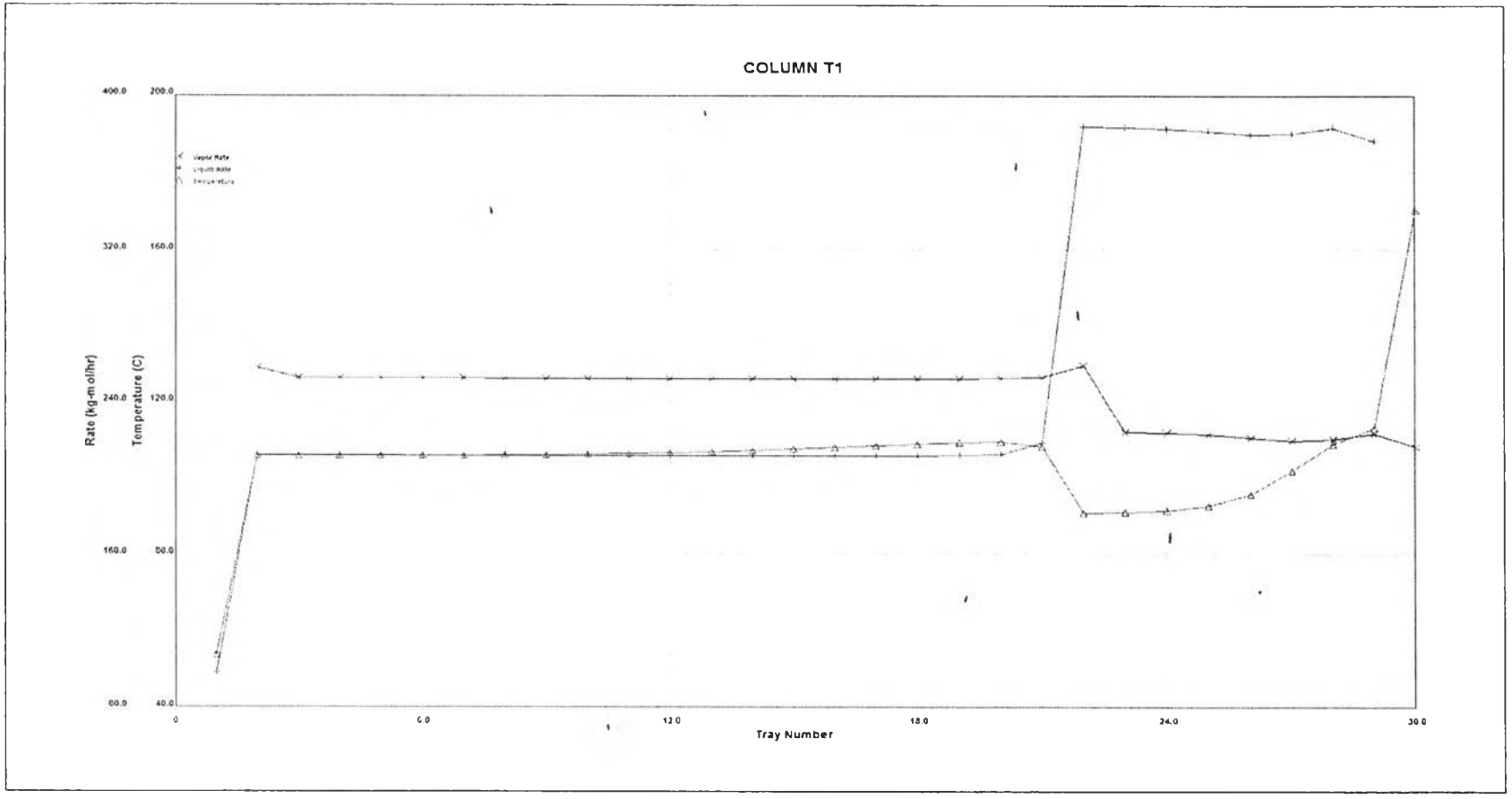

Figure D26 Overview of temperature and flowrate of the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

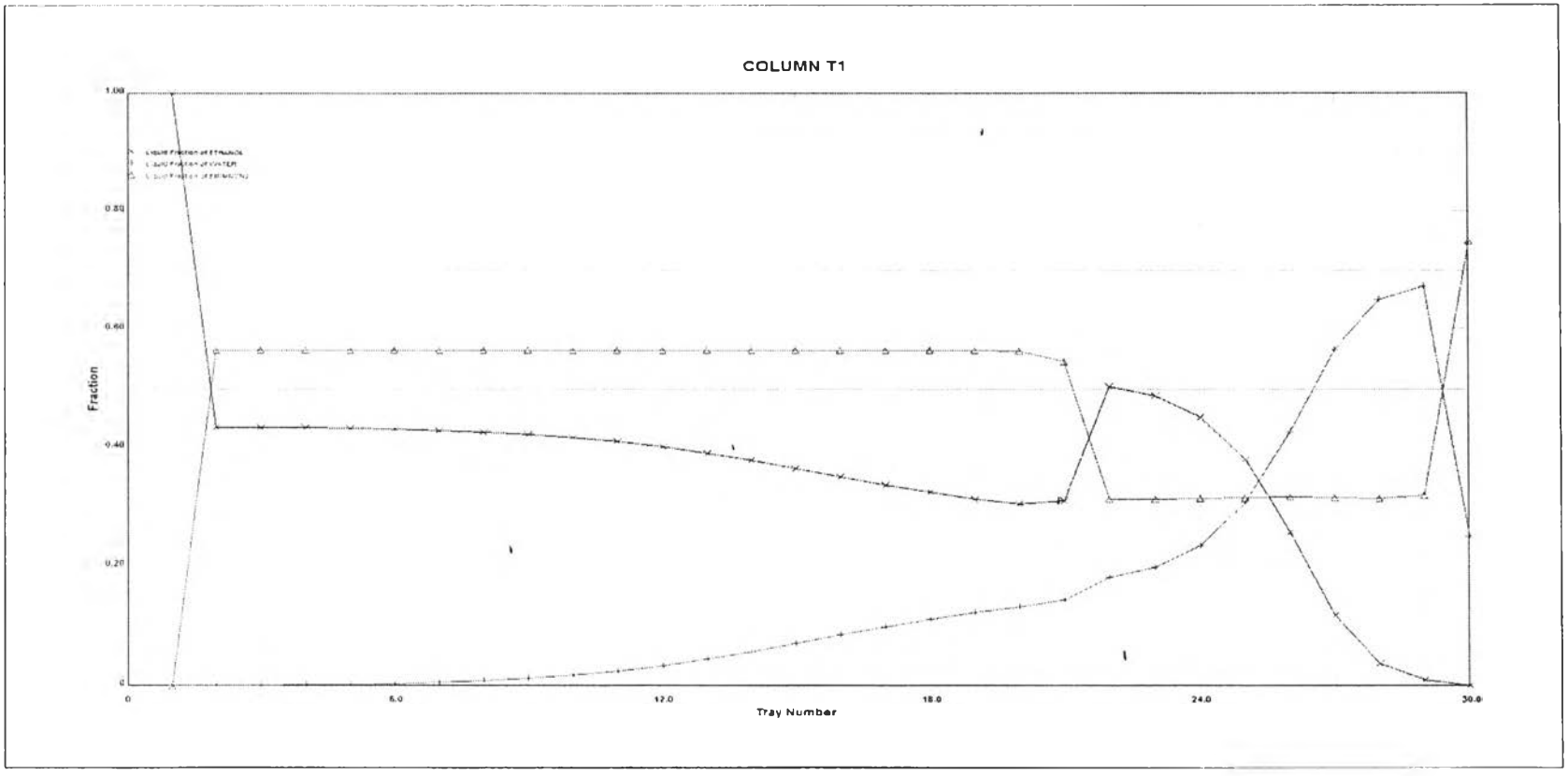

Figure D27 Overview of liquid fraction of the components in the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

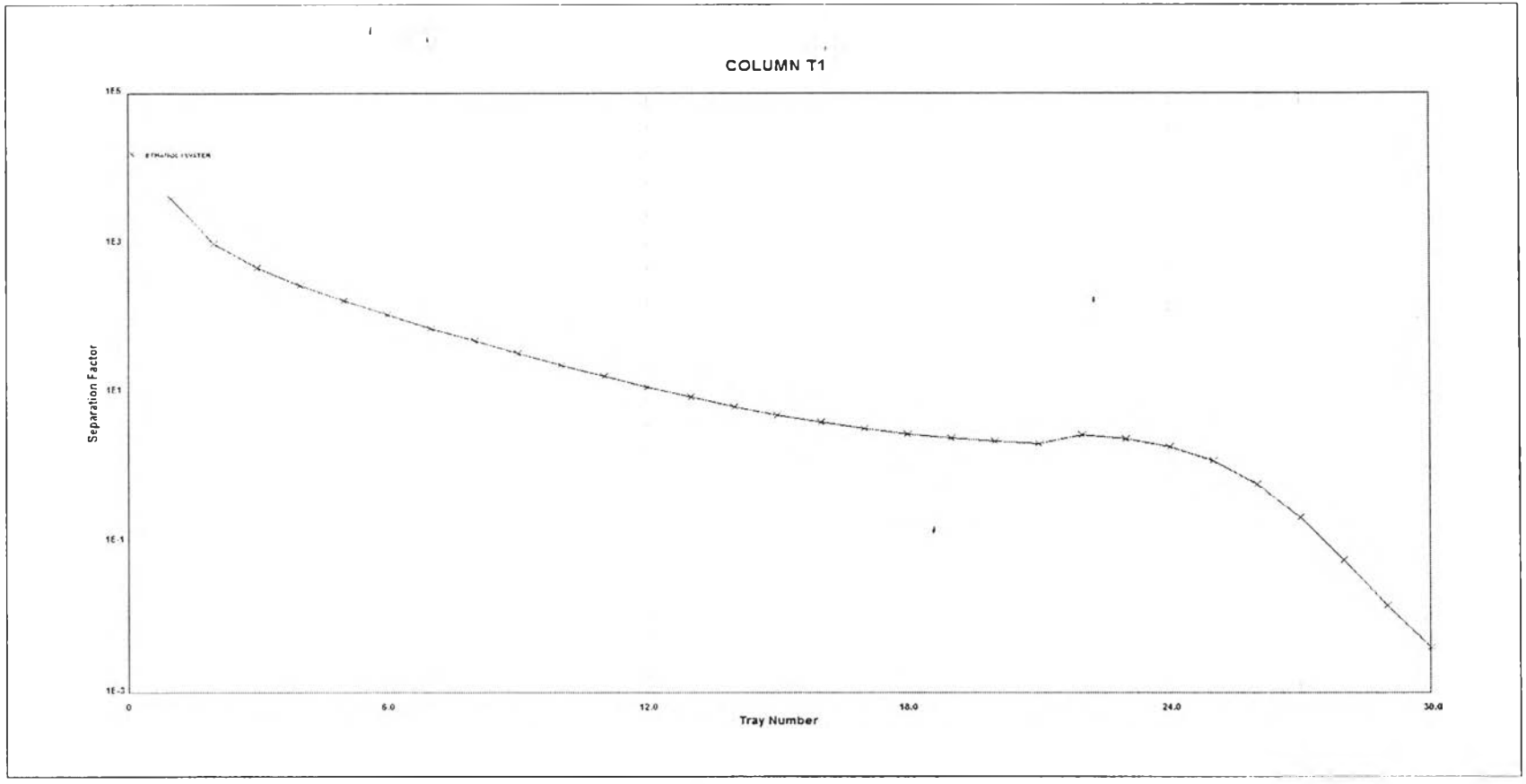

Figure D28 Separation factor in the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

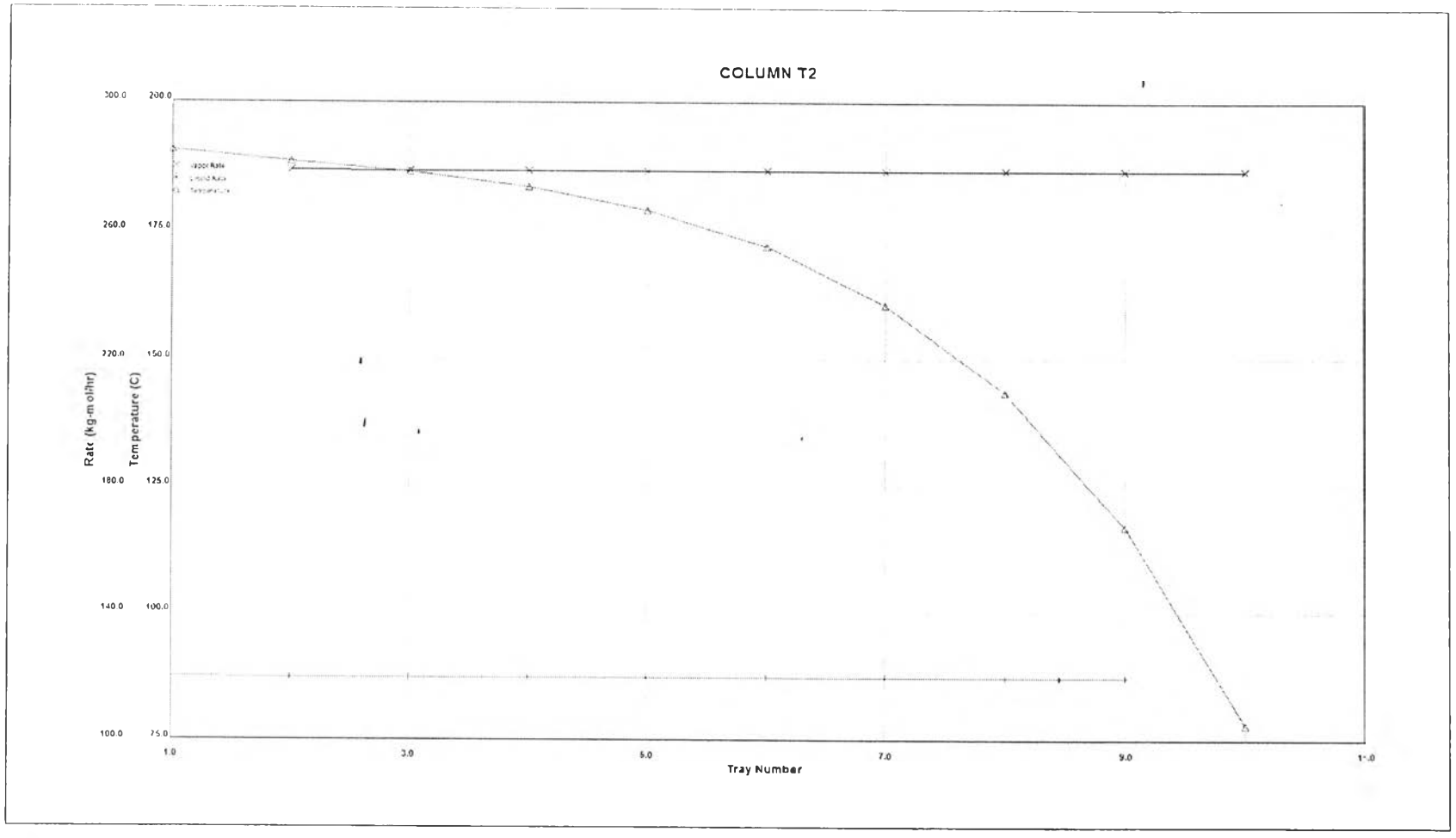

Figure D29 Overview of temperature and flowrate in the stripping column (column T2) using $[C_2mim][N(CN)_2]$ vs. tray number.

D.6 Optimal Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using [C_1mim][DMP]

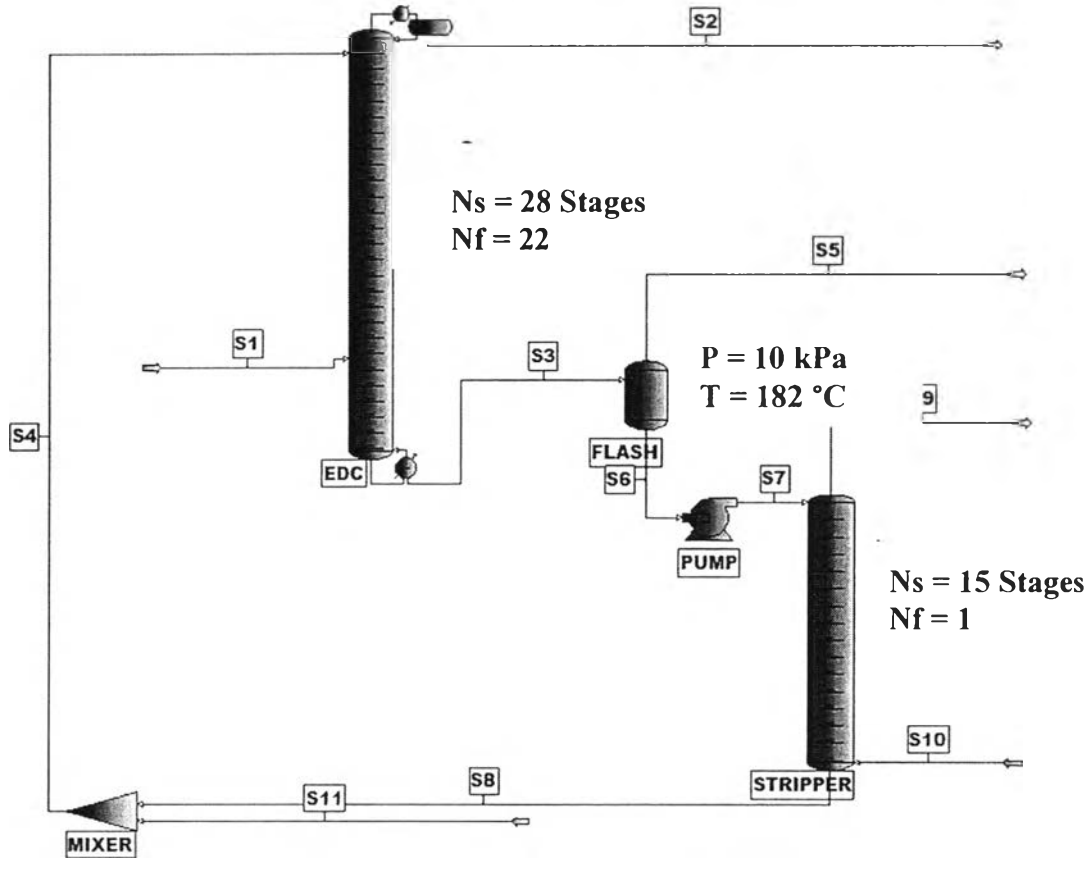

Figure D30 Extractive distillation process flowsheet using [C_1mim][DMP].

Table D19 Optimal extractive distillation column properties using [C_1mim][DMP]

Column Name	Unit	T1
Column Description		
Condenser Duty	MM WATT	-3.101
Reboiler Duty	MM WATT	3.1655
Column Total Molar Feed	KG-MOL/HR	253.4876
Column Total Wt. Feed	KG/HR	19959.2321
Column Condenser Pres	KPA	100
Column Condenser Temp	C	68.6588
Column Reflux Rate	KG-MOL/HR	103.2782
Column Reflux Ratio		0.646

Table D20 Flash properties of the optimal separation process using [C_1mim][DMP]

Flash Name	Unit	F1
Flash Description		
Temperature	C	182
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	0.4727

Table D21 Pump properties of the optimal separation process using [C_1mim][DMP]

Pump Name		P1
Pump Description		
Pressure Gain	KPA	90
Head	M	7.4136
Work	KW	0.3007

Table D22 Stream table of the optimal extractive distillation process using [C_1mim][DMP]

Stream Name		S1	S2	S3	S4	S5	S6	S10	S7	S8	S9
Stream Description											
Phase		Liquid	Liquid	Liquid	Liquid	Vapor	Liquid	Vapor	Liquid	Liquid	Vapor
Temperature	C	78.07	68.6588	169.9537	78.00844	182	182	25	182.1038	78.00907	165.2734
Pressure	KPA	100.00	100	100	100	10	10	100	100	100	100
Total Mass Rate	KG/HR	8092	7356	12603	11868	685	11919	2643	11919	11868	2694
Flowrate	KG-MOL/HR	200	160	94	53	37	56	91	56	53	94
Total Weight Comp. Rates	KG/HR										
ETHANOL		7371.05	7348.94	22.11	0.00	21.59	0.52	0.00	0.52	0.00	0.52
WATER		720.61	5.52	715.82	0.73	663.05	52.77	0.00	52.77	0.73	52.04
AIR		0.00	1.36	0.00	1.36	0.00	0.00	2643.09	0.00	1.36	2641.74
C1MIMDMP		0.00	0.00	11865.48	11865.48	0.00	11865.48	0.00	11865.48	11865.48	0.00
Total Weight Comp. Fractions											
ETHANOL		0.911	0.999	0.002	0.000	0.032	0.000	0.000	0.000	0.000	0.000
WATER		0.089	0.001	0.057	0.000	0.968	0.004	0.000	0.004	0.000	0.019
AIR		0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.980
C1MIMDMP		0.000	0.000	0.941	1.000	0.000	0.996	0.000	0.996	1.000	0.000
Total Molar Comp. Rates	KG-MOL/HR										
ETHANOL		160.00	159.5	0.5	0.0	0.5	0.0	0.0	0.0	0.0	0.0
WATER		40.00	0.3	39.7	0.0	36.8	2.9	0.0	2.9	0.0	2.9
AIR		0	0.0	0.0	0.0	0.0	0.0	91.3	0.0	0.0	91.2
C1MIMDMP		0	0.0	53.4	53.4	0.0	53.4	0.0	53.4	53.4	0.0
Composition											
ETHANOL		0.8	0.998	0.005	0.000	0.013	0.000	0.000	0.000	0.000	0.000
WATER		0.2	0.002	0.424	0.001	0.987	0.052	0.000	0.052	0.001	0.031
AIR		0	0.000	0.000	0.001	0.000	0.000	1.000	0.000	0.001	0.969
C1MIMDMP		0	0.000	0.570	0.998	0.000	0.948	0.000	0.948	0.998	0.000

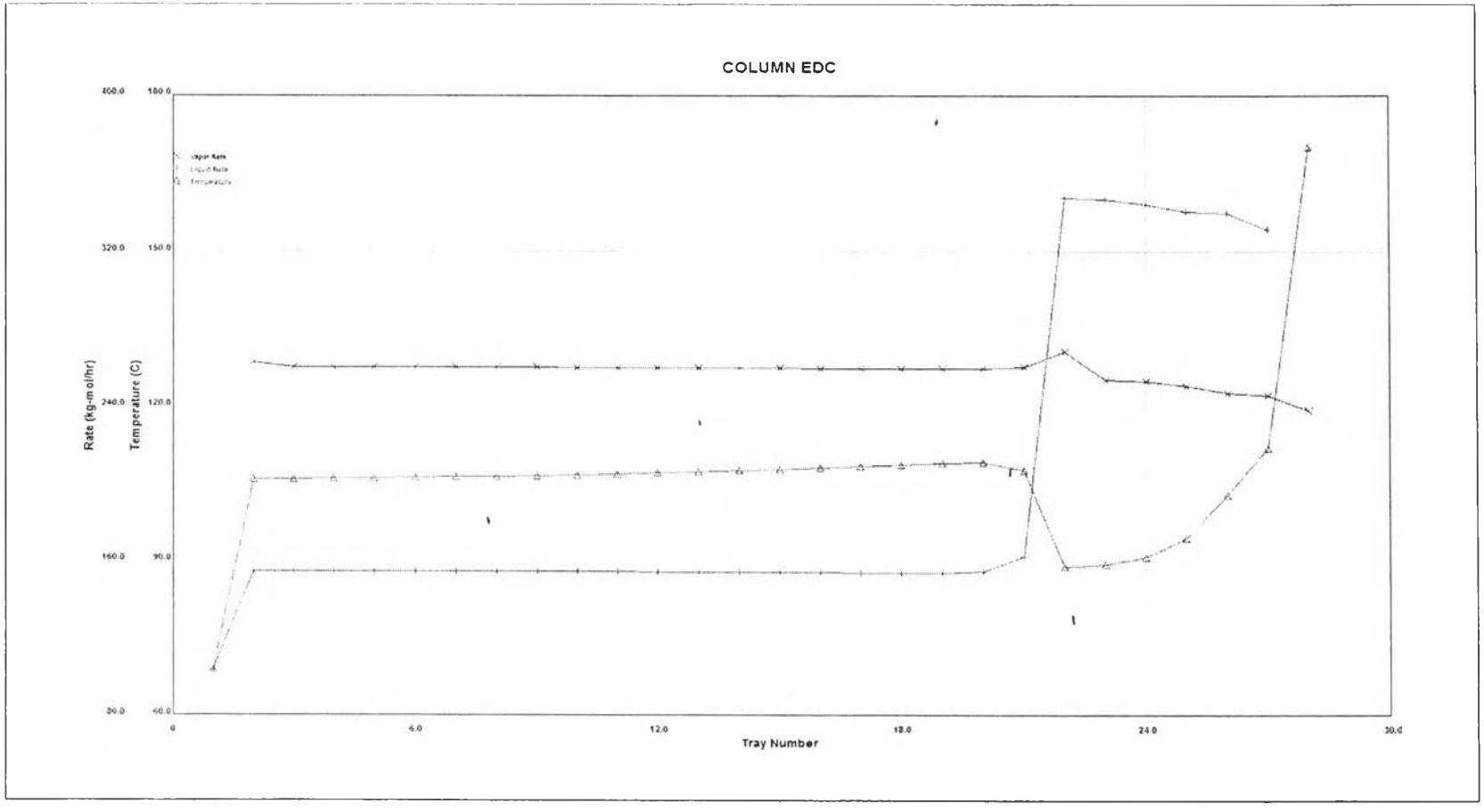

Figure D31 Overview of temperature and flowrate of the optimal extractive distillation process (column T1) using [C_1mim][DMP] vs. tray number.

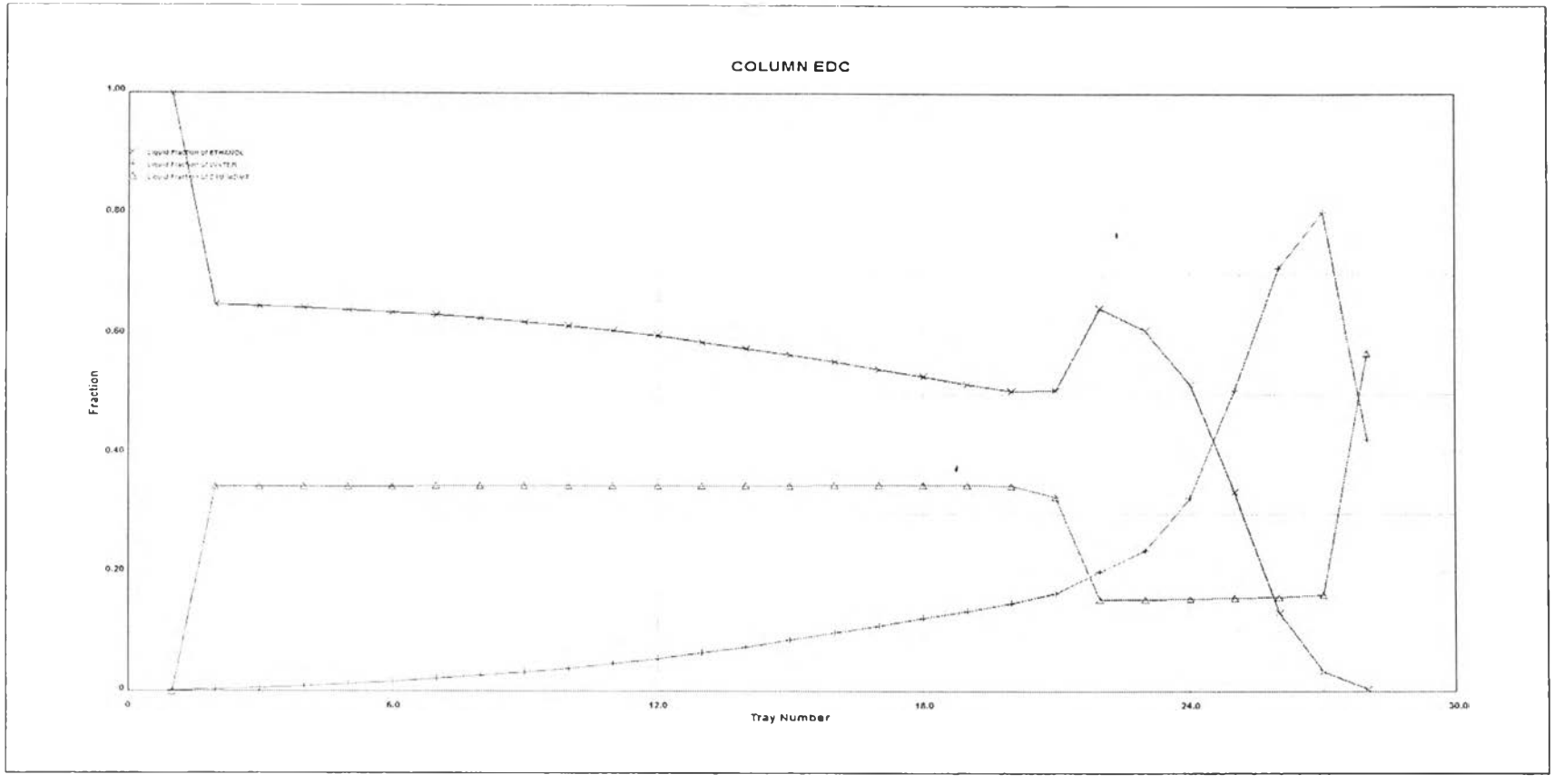

Figure D32 Overview of temperature and flowrate of the optimal extractive distillation process (column T1) using $[C_1mim][DMP]$ vs. tray number.

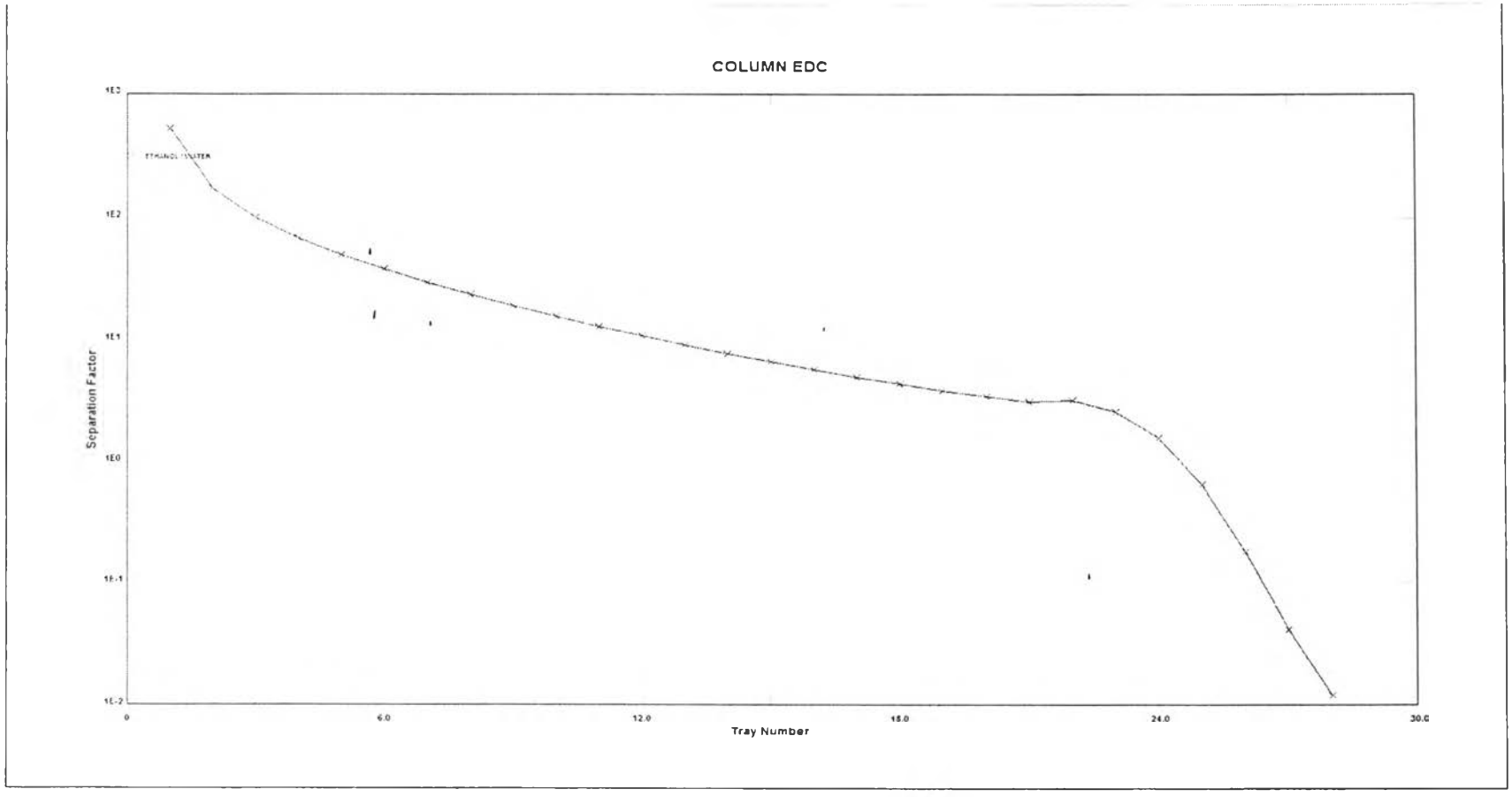

Figure D33 Separation factor in the optimal extractive distillation process (column T1) using $[C_1mim][DMP]$ vs. tray number.

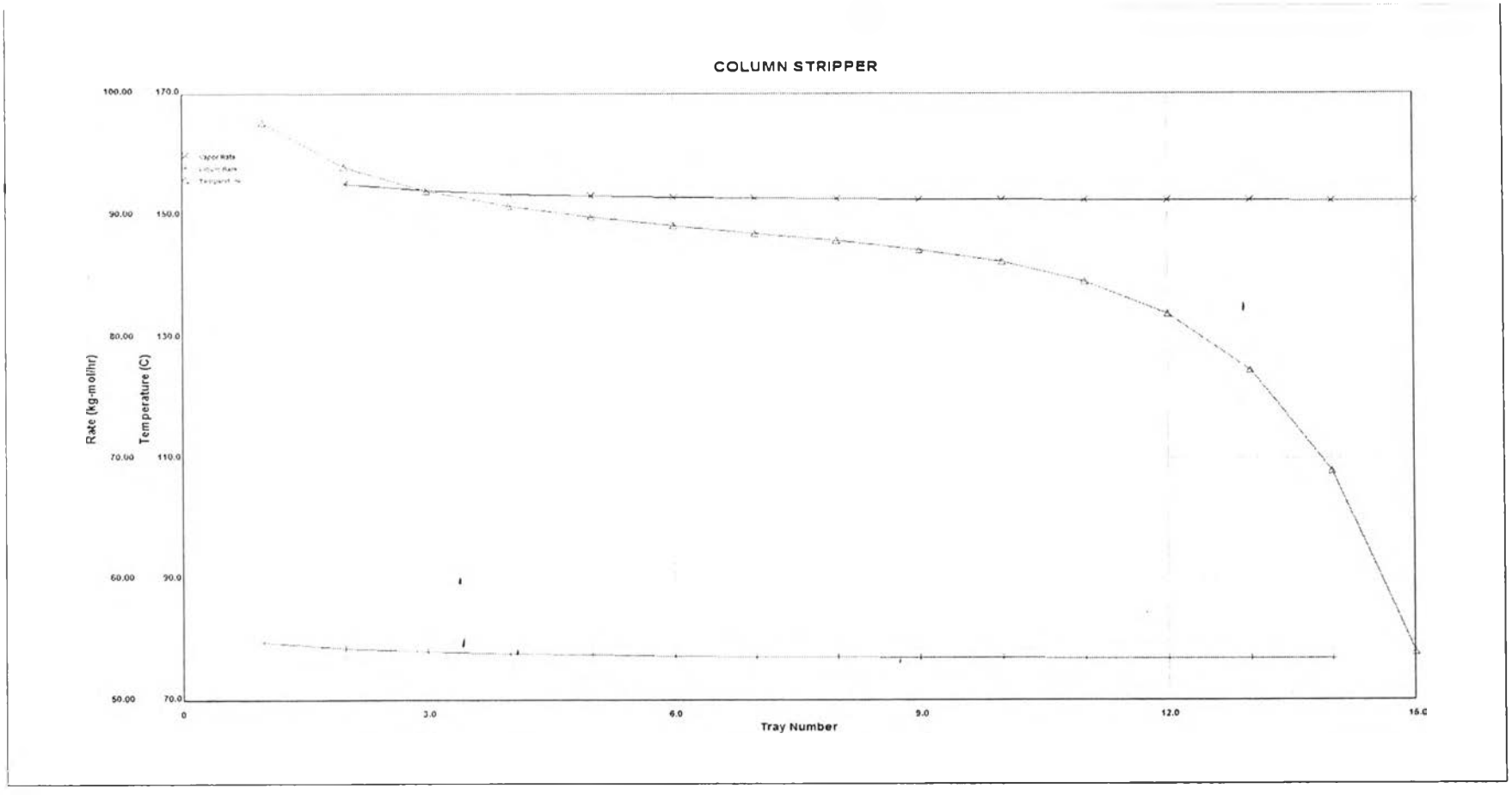

Figure D34 Overview of temperature and flowrate in the optimal stripping column (column T2) using **[**C_1mim][DMP] vs. tray number.

D.7 Extractive Distillation Process Flowsheet for Isopropanol + Water Separation Using [C_1mim][DMP]

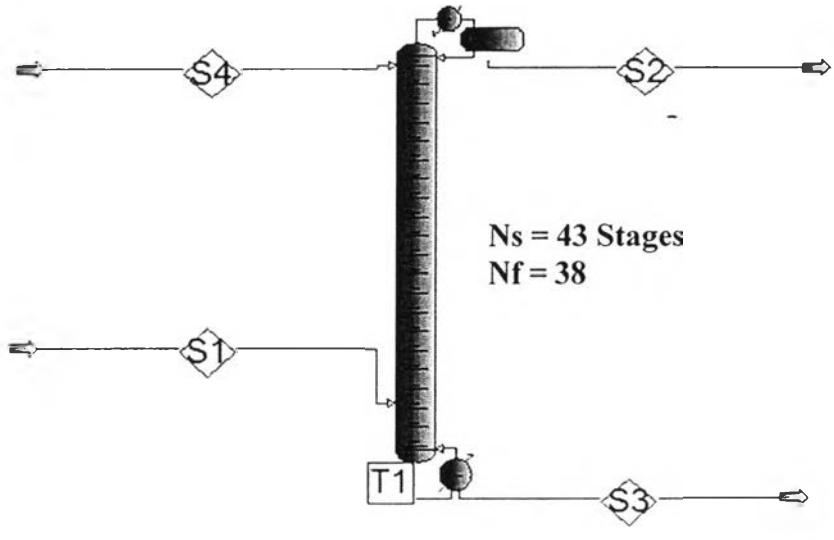

Figure D35 Extractive distillation process flowsheet using [C_1mim][DMP].

Table D23 Extractive distillation column properties using [C_1mim][DMP]

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-6.1474
Reboiler Duty	MM WATT	6.8175
Column Total Molar Feed	KG-MOL/HR	410.0002
Column_Total Wt. Feed	KG/HR	55228.9817
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	81.9782
Column Reflux Rate	KG-MOL/HR	421.5434
Column Reflux Ratio		3.5006

Table D24 Stream table of the extractive distillation process using [C_1mim][DMP]

Stream Name		S1	S2	S3	S4
Stream Description					
Phase		Liquid	Liquid	Liquid	Liquid
Temperature	C	79.7519	81.9782	196.3137	80.0000
Pressure	KPA	100.0000	100.0000	100.0000	100.0000
Total Mass Rate	KG/HR	8652.7399	7208.9850	48019.9967	46576.2418
Flowrate	KGMOL/HR	200.0002	120.4202	289.5799	210.0000
Total Weight Comp. Rates	KG/HR				
WATER		1441.2236	11.8930	1436.8970	7.5664
AIR		0.0000	0.0000	0.0000	0.0000
IPRPALC		7211.5163	7197.0920	14.4243	0.0000
C1MIMDMP		0.0000	0.0000	46568.6754	46568.6754
Total Weight Comp. Fractions					
WATER		0.1666	0.0016	0.0299	0.0002
AIR		0.0000	0.0000	0.0000	0.0000
IPRPALC		0.8334	0.9984	0.0003	0.0000
C1MIMDMP		0.0000	0.0000	0.9698	0.9998
Total Molar Comp. Rates	KGMOL/HR				
WATER		80.0001	0.6602	79.7599	0.4200
AIR		0.0000	0.0000	0.0000	0.0000
IPRPALC		120.0001	119.7601	0.2400	0.0000
C1MIMDMP		0.0000	0.0000	209.5800	209.5800
Composition					
WATER		0.4000	0.0055	0.2754	0.0020
AIR		0.0000	0.0000	0.0000	0.0000
IPRPALC		0.6000	0.9945	0.0008	0.0000
C1MIMDMP		0.0000	0.0000	0.7237	0.9980

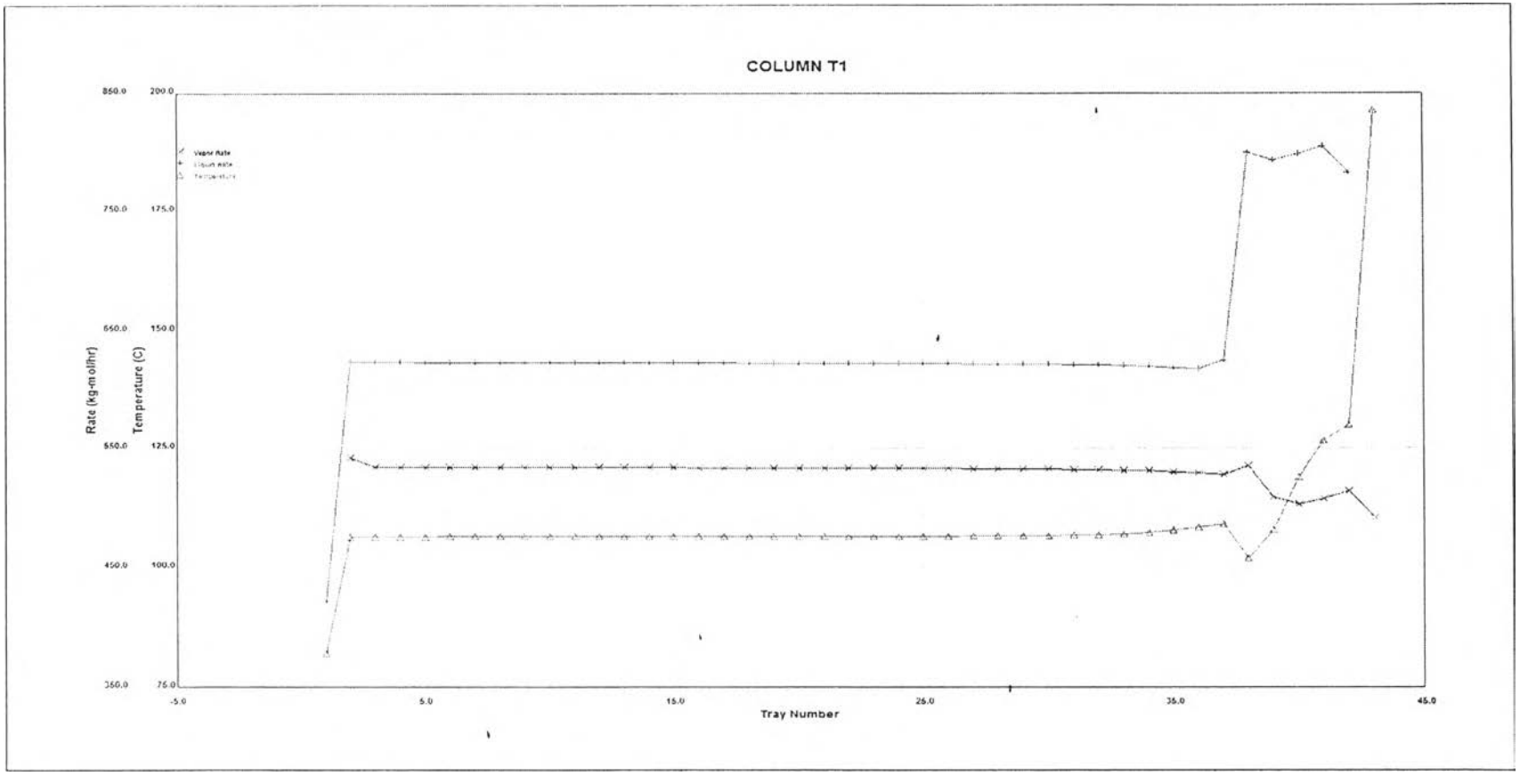

Figure D36 Overview of temperature and flowrate of the extractive distillation process (column T1) using $[C_1mim][DMP]$ vs. tray number.

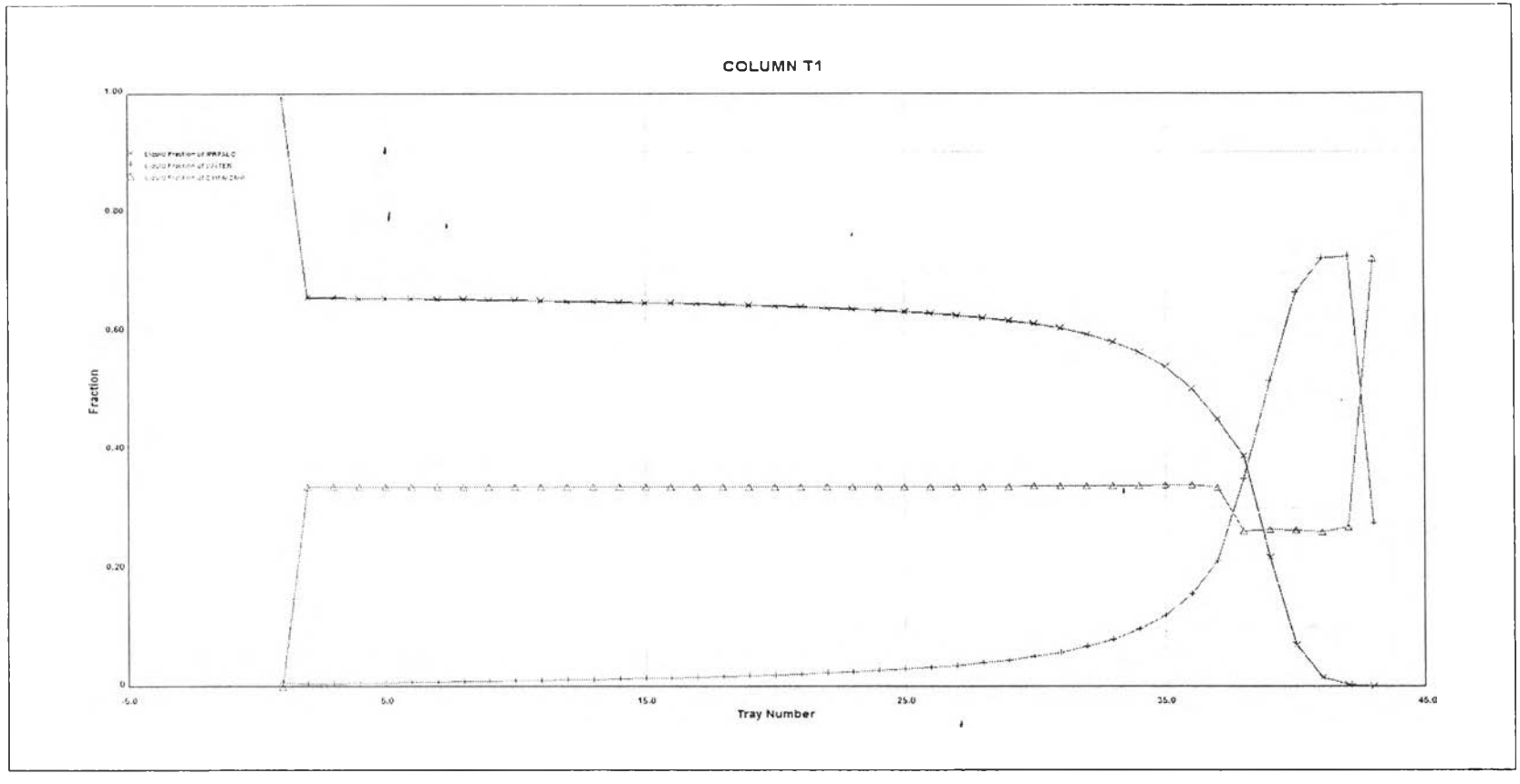

Figure D37 Overview of liquid fraction of the components in the extractive distillation process (column T1) using [C_1mim][DMP] vs. tray number.

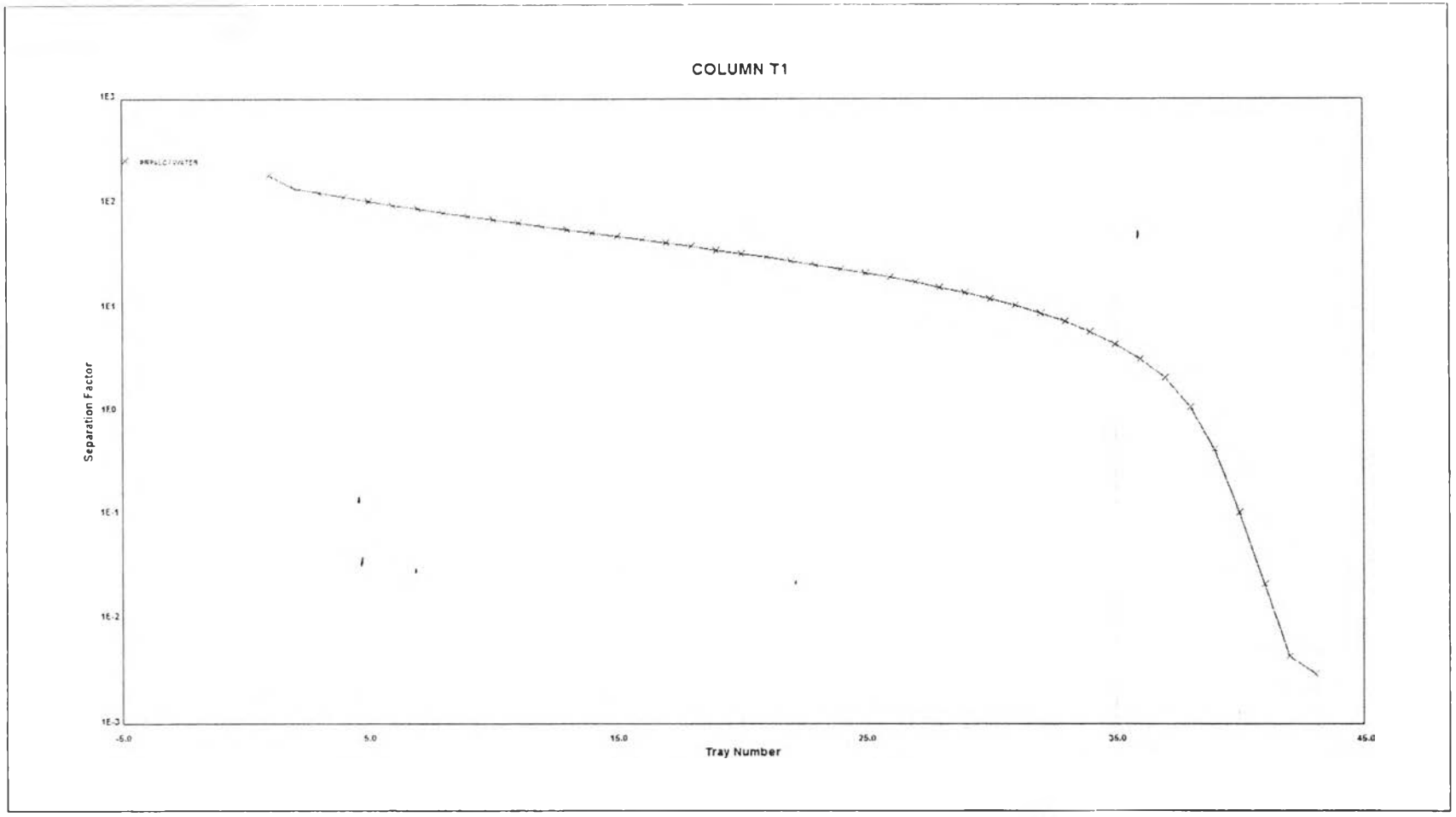

Figure D38 Separation factor in the extractive distillation process (column T1) using [C_1mim][DMP] vs. tray number

D.8 Extractive Distillation Process Flowsheet for Isopropanol + Water Separation Using [C_2mim][$N(CN)_2$] Fixed Condition As Ethanol + Water Separation

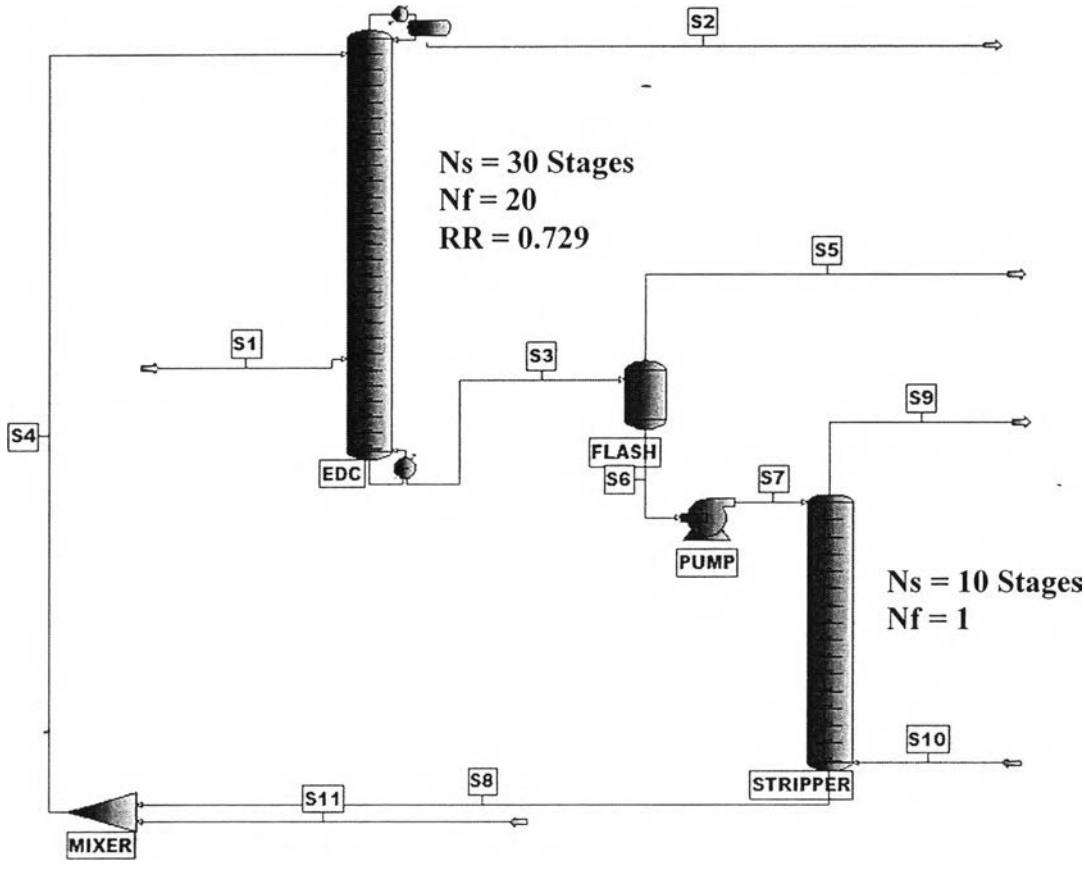

Figure D39 Extractive distillation process flowsheet using [C_2mim][$N(CN)_2$].

Table D25 Extractive distillation column properties using $[C_2mim][N(CN)_2]$

Column Name	Unit	T1
Condenser Duty	MM WATT	-2.7219
Reboiler Duty	MM WATT	2.5441
Column Total Molar Feed	KG-MOL/HR	320.1054
Column Total Wt. Feed	KG/HR	29919.79
Column Condenser Pres	KPA	100
Column Condenser Temp	C	45.2926
Column Reflux Rate	KG-MOL/HR	87.1131
Column Reflux Ratio		0.7287

Table D26 Flash properties of the separation process using $[C_2mim][N(CN)_2]$

Flash Name	Unit	F1
Flash Description		
Temperature	C	200
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	1.3373

Table D27 Pump properties of the separation process using $[C_2mim][N(CN)_2]$

Pump Name		P1
Pump Description		
Pressure Gain	KPA	90
Head	M	8.7377
Work	KW	0.6335

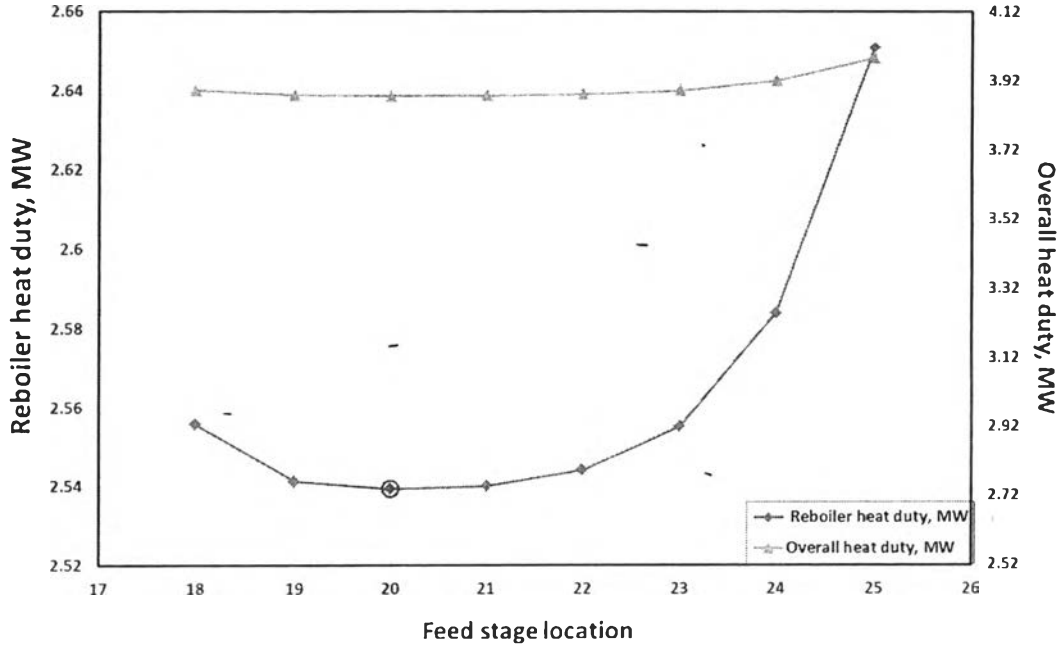

Figure D40 Reboiler heat duty and overall heat duty as a function of feed stage location for separation of the ethanol + water azeotrope using $[C_2mim][N(CN)_2]$= 120 kg-mol/hr (fixed Ns=30 stages, Nf = 20).

Table D28 Stream table of the extractive distillation process using $[C_2mim][N(CN)_2]$

Stream Name		S1	S2	S3	S5	S6	S10	S7	S9	S8	S11	S4
Stream Description												
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Liquid	Liquid
Temperature	C	79.75	45.26	138.41	168.00	168.00	25.00	168.04	153.11	78.00	78.00	78.00
Pressure	KPA	100.00	100.00	100.00	10.00	10.00	100.00	100.00	100.00	100.00	100.00	100.00
Total Mass Rate	KG/HR	8652	7174.77	22745.61	1385	21360	6192	21360	6285.	21267	n/a	21267
Flowrate	KGMOL/HR	200.00	119.58	200.56	75.22	125.34	213.84	125.34	219.04	120.14	-0.16	120.14
Total Weight Comp. Rates	KG/HR											
WATER		1441.22	3.48	1438.34	1342.25	96.09	0.00	96.09	95.50	0.59	0.00	0.59
AIR		0.00	3.05	0.00	0.00	0.00	6192.68	0.00	6189.63	3.05	0.00	3.05
IPRPALC		7211.52	7168.25	43.27	42.82	0.45	0.00	0.45	0.45	0.00	0.00	0.00
EMIMNCN2		0.00	0.00	21264	0.00	21264	0.00	21264	0.00	21264	-27.97	21264
Total Weight Comp. Fractions												
WATER		0.17	0.00	0.06	0.97	0.00	0.00	0.00	0.02	0.00	0.00	0.00
AIR		0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.98	0.00	0.00	0.00
IPRPALC		0.83	1.00	0.00	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EMIMNCN2		0.00	0.00	0.93	0.00	1.00	0.00	1.00	0.00	1.00	1.00	1.00
Total Molar Comp. Rates	KG-MOL/HR											
WATER		80.00	0.19	79.84	74.51	5.33	0.00	5.33	5.30	0.03	0.00	0.03
AIR		0.00	0.11	0.00	0.00	0.00	213.84	0.00	213.73	0.11	0.00	0.11
IPRPALC		120.00	119.28	0.72	0.71	0.01	0.00	0.01	0.01	0.00	0.00	0.00
EMIMNCN2		0.00	0.00	120.00	0.00	120.00	0.00	120.00	0.00	120.00	-0.16	120.00
Composition												
WATER		0.400	0.002	0.398	0.991	0.043	0.000	0.043	0.024	0.000	0.000	0.000
AIR		0.000	0.001	0.000	0.000	0.000	1.000	0.000	0.976	0.001	0.000	0.001
IPRPALC		0.600	0.998	0.004	0.009	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EMIMNCN2		0.000	0.000	0.598	0.000	0.957	0.000	0.957	0.000	0.999	1.000	0.999

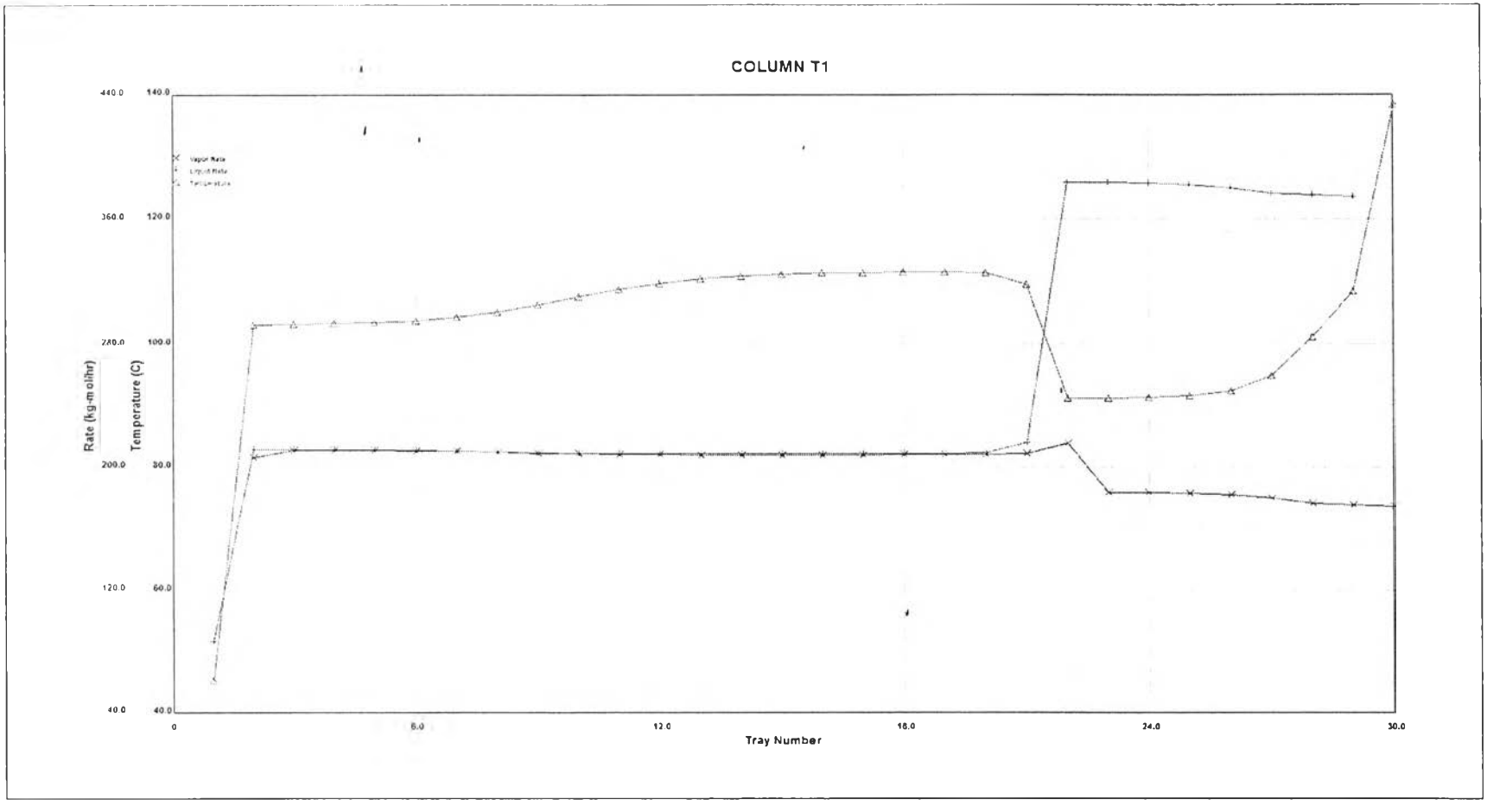

Figure D41 Overview of temperature and flowrate of the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

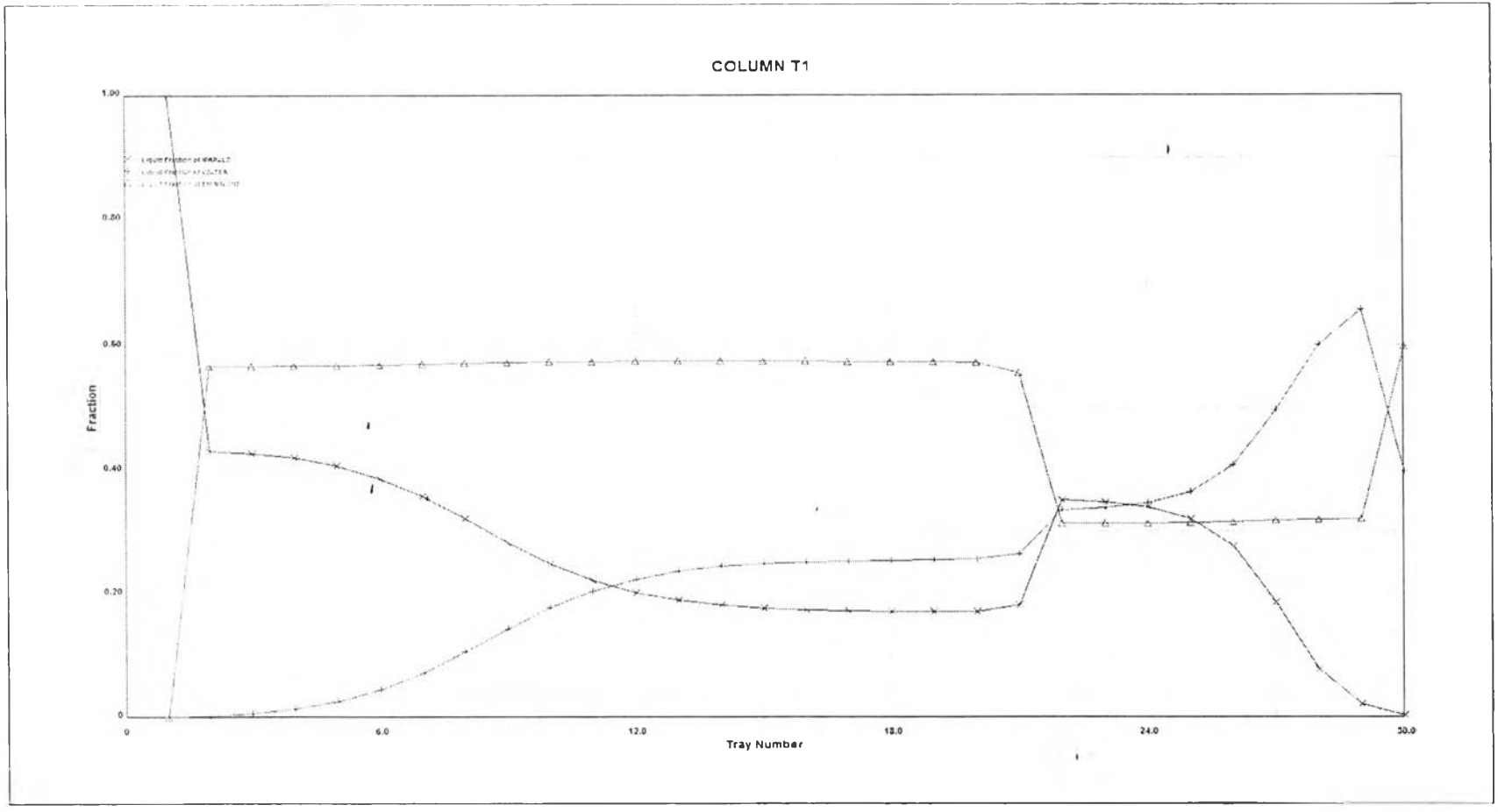

Figure D42 Overview of liquid fraction of the components in the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

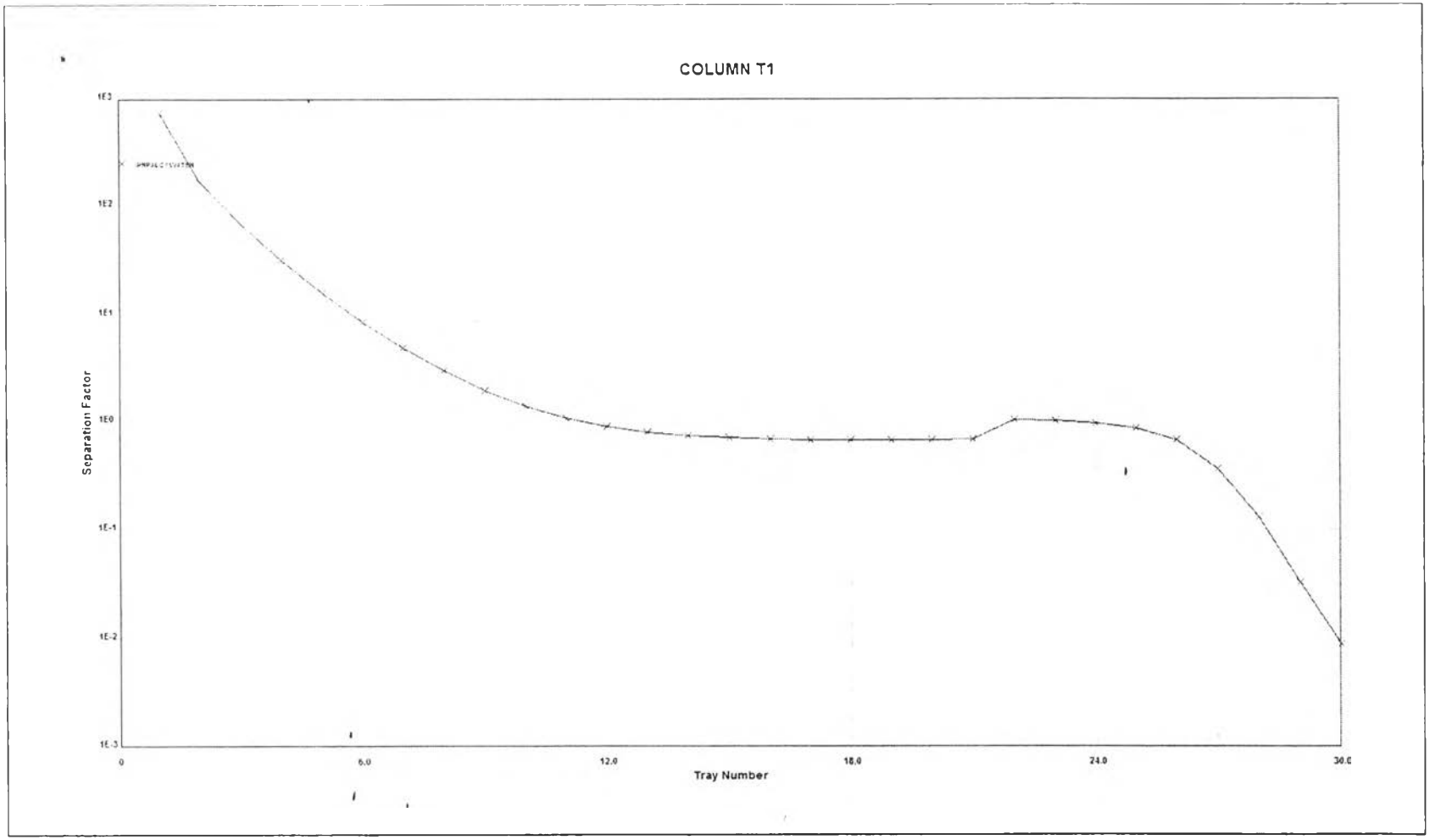

Figure D43 Separation factor in the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

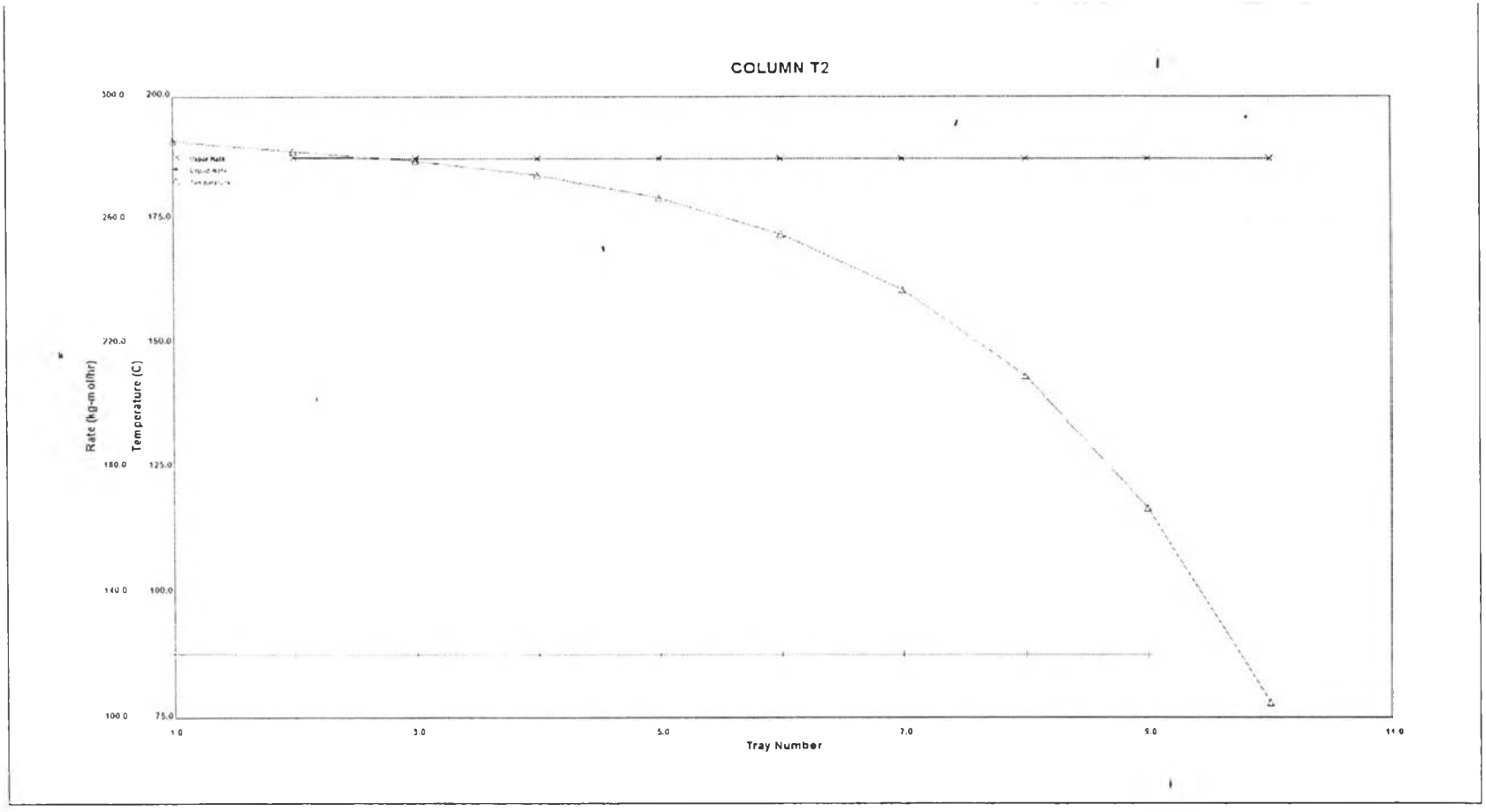

Figure D44 Overview of temperature and flowrate in the stripping column (column T2) using $[C_2mim][N(CN)_2]$ vs. tray number.

D.9 Extractive Distillation Process Flowsheet for Ethanol + Water Separation Using [C_2mim][$N(CN)_2$] Fixed Reflux Ratio equal to 0.729

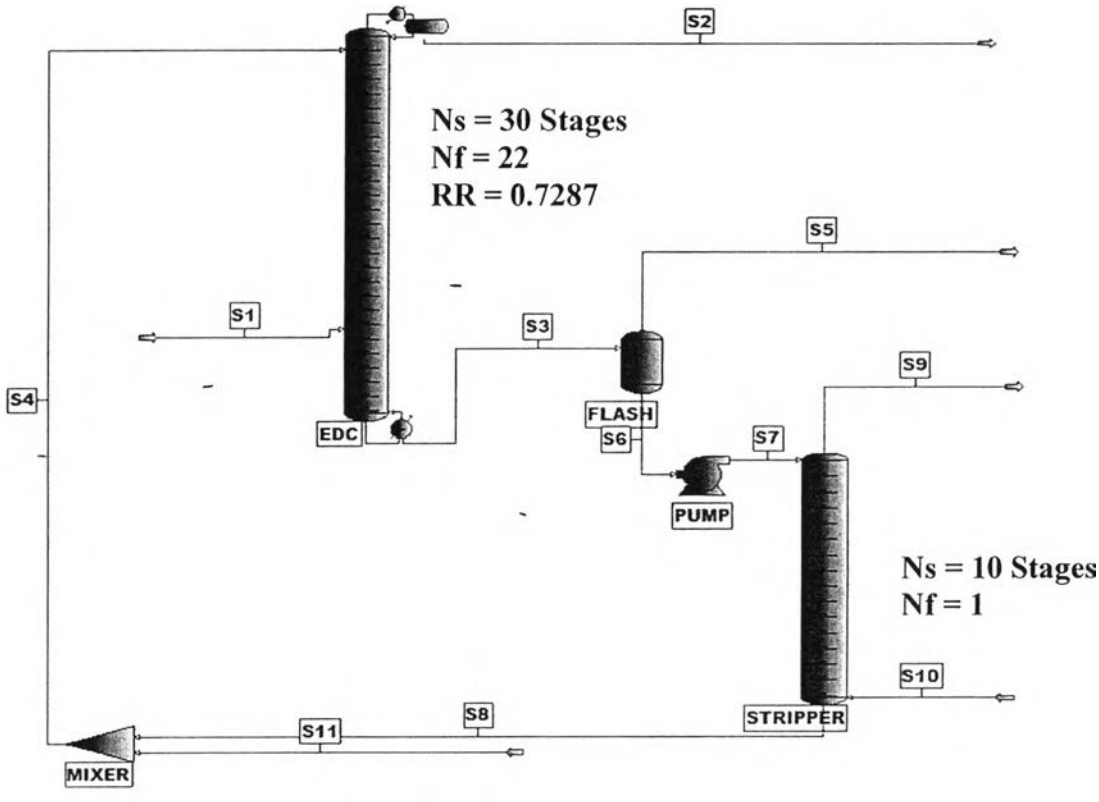

Figure D45 Extractive distillation process flowsheet using [C_2mim][$N(CN)_2$].

Table D29 Extractive distillation column properties using [C_2mim][$N(CN)_2$]

Column Name	Unit	T1
Condenser Duty	MM WATT	-3.423
Reboiler Duty	MM WATT	3.5136
Column Total Molar Feed	KG-MOL/HR	320.1054
Column Total Wt. Feed	KG/HR	29358.7103
Column Condenser Pres	KPA	100
Column Condenser Temp	C	53.845
Column Reflux Rate	KG-MOL/HR	116.6057
Column Reflux Ratio		0.729

Table D30 Flash properties of the separation process using $[C_2mim][N(CN)_2]$

Flash Name	Unit	F1
Flash Description		
Temperature	C	200
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	0.6185

Table D31 Pump properties of the separation process using $[C_2mim][N(CN)_2]$

Pump Name		P1
Pump Description		
Pressure Gain	KPA	90
Head	M	8.7377
Work	KW	0.6335

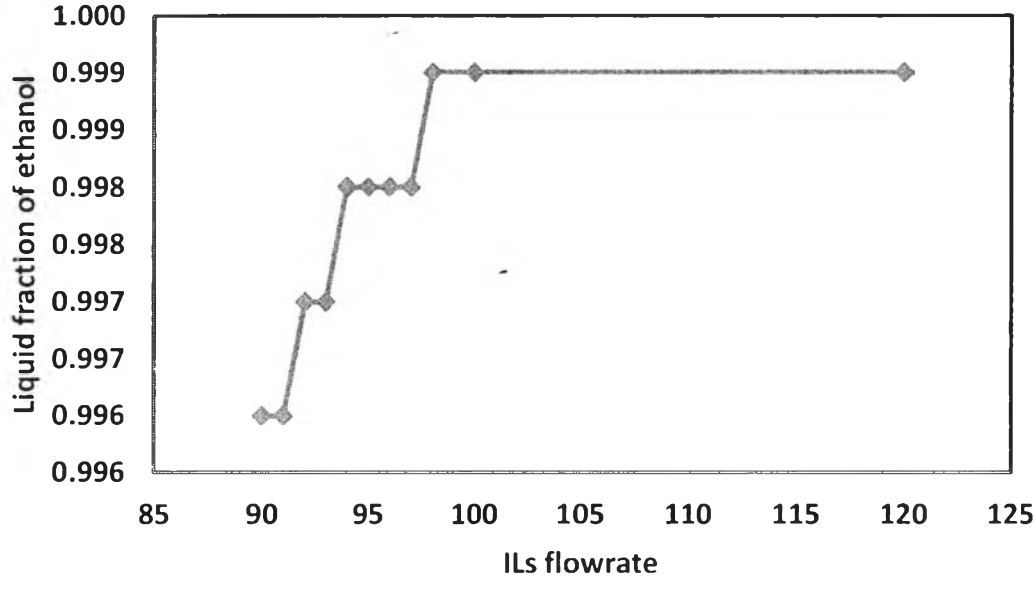

Figure D46 Comparison of the flowrate of $[C_2MIM][N(CN)_2]$ versus liquid molar fraction of the ethanol in EDC.

Table D32 Stream table of the extractive distillation process using $[C_2mim][N(CN)_2]$

Stream Name		S1	S2	S3	S5	S6	S7	S8	S10	S11	S4	S9
Stream Description												
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Vapor
Temperature	C	78	54	170	200	200	200	78	25	78	78	191
Pressure	KPA	100	100	100	10	10	100	100	100	100	100	100
Total Mass Rate	KG/HR	8091.66	7366.87	21991.84	682.76	21309.08	21309.08	21267.05	8087.28	n/a	21267.05	8129.31
Flowrate	KG-MOL/HR	200.00	159.95	160.15	37.65	122.50	122.50	120.11	279.26	-0.14	120.11	281.65
Total Weight Comp. Rates	KG/HR											
ETHANOL		7371.05	7363.68	7.37	7.27	0.10	0.10	0.00	0.00	0.00	0.00	0.10
WATER		720.61	0.14	720.47	675.49	44.98	44.98	0.00	0.00	0.00	0.00	44.98
AIR		0.00	3.05	0.00	0.00	0.00	0.00	3.05	8087.28	0.00	3.05	8084.23
EMIMNCN2		0.00	0.00	21264.00	0.00	21264.00	21264.00	21264.00	0.00	-24.87	21264.00	0.00
Total Weight Comp. Fractions												
ETHANOL		0.911	1.000	0.000	0.011	0.000	0.000	0.000	0.000	0.000	0.000	0.000
WATER		0.089	0.000	0.033	0.989	0.002	0.002	0.000	0.000	0.000	0.000	0.006
AIR		0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000	0.000	0.000	0.994
EMIMNCN2		0.000	0.000	0.967	0.000	0.998	0.998	1.000	0.000	1.000	1.000	0.000
Total Molar Comp. Rates	KG-MOL/HR											
ETHANOL		160.000	159.840	0.160	0.158	0.002	0.002	0.000	0.000	0.000	0.000	0.002
WATER		40.000	0.008	39.992	37.496	2.497	2.497	0.000	0.000	0.000	0.000	2.497
AIR		0.000	0.105	0.000	0.000	0.000	0.000	0.105	279.257	0.000	0.105	279.152
EMIMNCN2		0.000	0.000	120.000	0.000	120.000	120.000	120.000	0.000	-0.140	120.000	0.000
Composition												
ETHANOL		0.800	0.999	0.001	0.004	0.000	0.000	0.000	0.000	0.000	0.000	0.000
WATER		0.200	0.000	0.250	0.996	0.020	0.020	0.000	0.000	0.000	0.000	0.009
AIR		0.000	0.001	0.000	0.000	0.000	0.000	0.001	1.000	0.000	0.001	0.991
EMIMNCN2		0.000	0.000	0.749	0.000	0.980	0.980	0.999	0.000	1.000	0.999	0.000

D.10 Optimal Extractive Distillation Process Flowsheet for Isopropanol + Water Separation Using $[C_2mim][N(CN)_2]$

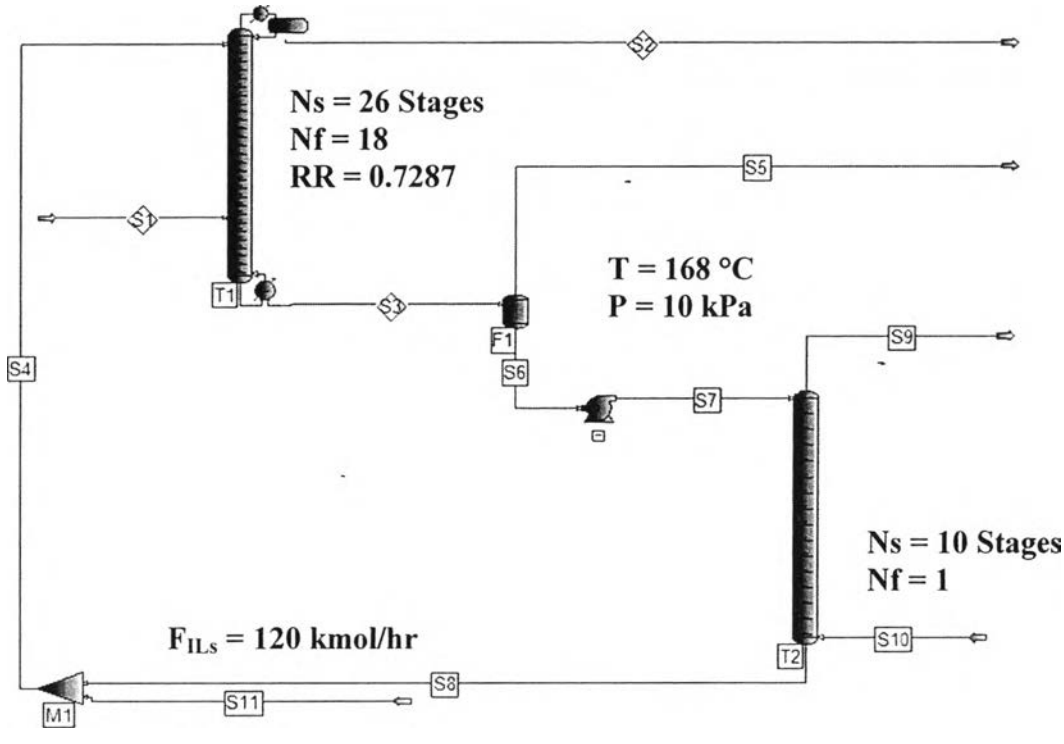

Figure D47 Extractive distillation process flowsheet using $[C_2mim][N(CN)_2]$.

Table D33 Optimal extractive distillation column properties using $[C_2mim][N(CN)_2]$

Column Name		**T1**
Column Description		
Condenser Duty	MM WATT	-2.7137
Reboiler Duty	MM WATT	2.5305
Column Total Molar Feed	KG-MOL/HR	320.1374
Column Total Wt. Feed	KG/HR	29920.3625
Column Condenser Pres	KPA	100
Column Condenser Temp	C	45.125
Column Reflux Rate	KG-MOL/HR	86.7855
Column Reflux Ratio		0.7287

Table D34 Flash properties of the optimal separation process using $[C_2mim][N(CN)_2]$

Flash Name		**F1**
Temperature	C	168
Pressure	KPA	10
DP	KPA	90
Duty	MM WATT	1.1684

Table D35 Pump properties of the optimal separation process using $[C_2mim][N(CN)_2]$

Pump Name		**P1**
Pump Description		
Pressure Gain	KPA	90
Head	M	8.7377
Work	KW	0.6335

Table D36 Stream table of the optimal extractive distillation process using $[C_2mim][N(CN)_2]$

Stream Name		S1	S2	S3	S5	S6	S10	S7	S9	S8	S11	S4
Stream Description												
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Vapor	Liquid	Vapor	Liquid	Liquid	Liquid
Temperature	C	79.75	45.12	137.47	168.00	168.00	25.00	168.04	153.16	78.01	78.00	78.02
Pressure	KPA	100.00	100.00	100.00	10.00	10.00	100.00	100.00	100.00	100.00	100.00	100.00
Total Mass Rate	KG/HR	8652.74	7145.89	22774.47	1414.19	21360.28	6198.53	21360.28	6291.19	21267.62	n/a	21267.62
Flowrate	KGMOL/HR	200.00	119.10	201.04	75.73	125.32	214.04	125.32	219.22	120.14	-0.21	120.14
Total Weight Comp. Rates	KG/HR											
WATER		1441.22	3.44	1438.36	1342.81	95.55	0.00	95.55	94.97	0.58	0.00	0.58
AIR		0.00	3.05	0.00	0.00	0.00	6198.53	0.00	6195.48	3.05	0.00	3.05
IPRPALC		7211.52	7139.40	72.12	71.38	0.74	0.00	0.74	0.74	0.00	0.00	0.00
EMIMNCN2		0.00	0.00	21264.00	0.00	21264.00	0.00	21264.00	0.00	21264.00	-36.46	21264.00
Total Weight Comp. Fractions												
WATER		0.17	0.00	0.06	0.95	0.00	0.00	0.00	0.02	0.00	0.00	0.00
AIR		0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.98	0.00	0.00	0.00
IPRPALC		0.83	1.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00
EMIMNCN2		0.00	0.00	0.93	0.00	1.00	0.00	1.00	0.00	1.00	1.00	1.00
Total Molar Comp. Rates	KGMOL/HR											
WATER		80.00	0.19	79.84	74.54	5.30	0.00	5.30	5.27	0.03	0.00	0.03
AIR		0.00	0.11	0.00	0.00	0.00	214.04	0.00	213.93	0.11	0.00	0.11
IPRPALC		120.00	118.80	1.20	1.19	0.01	0.00	0.01	0.01	0.00	0.00	0.00
EMIMNCN2		0.00	0.00	120.00	0.00	120.00	0.00	120.00	0.00	120.00	-0.21	120.00
Composition												
WATER		0.400	0.002	0.397	0.984	0.042	0.000	0.042	0.024	0.000	0.000	0.000
AIR		0.000	0.001	0.000	0.000	0.000	1.000	0.000	0.976	0.001	0.000	0.001
IPRPALC		0.600	0.998	0.006	0.016	0.000	0.000	0.000	0.000	0.000	0.000	0.000
EMIMNCN2		0.000	0.000	0.597	0.000	0.958	0.000	0.958	0.000	0.999	1.000	0.999

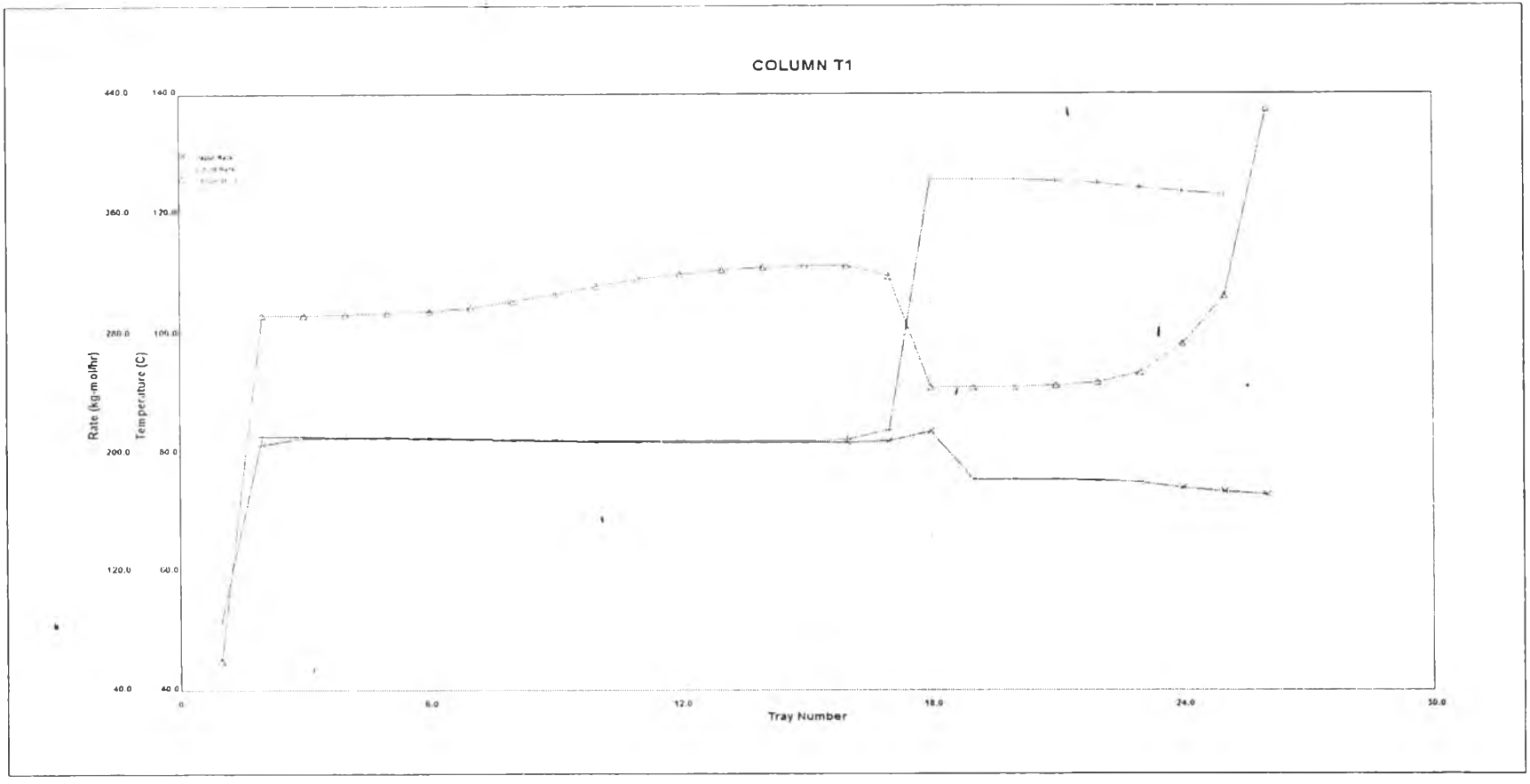

Figure D48 Overview of temperature and flowrate of the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

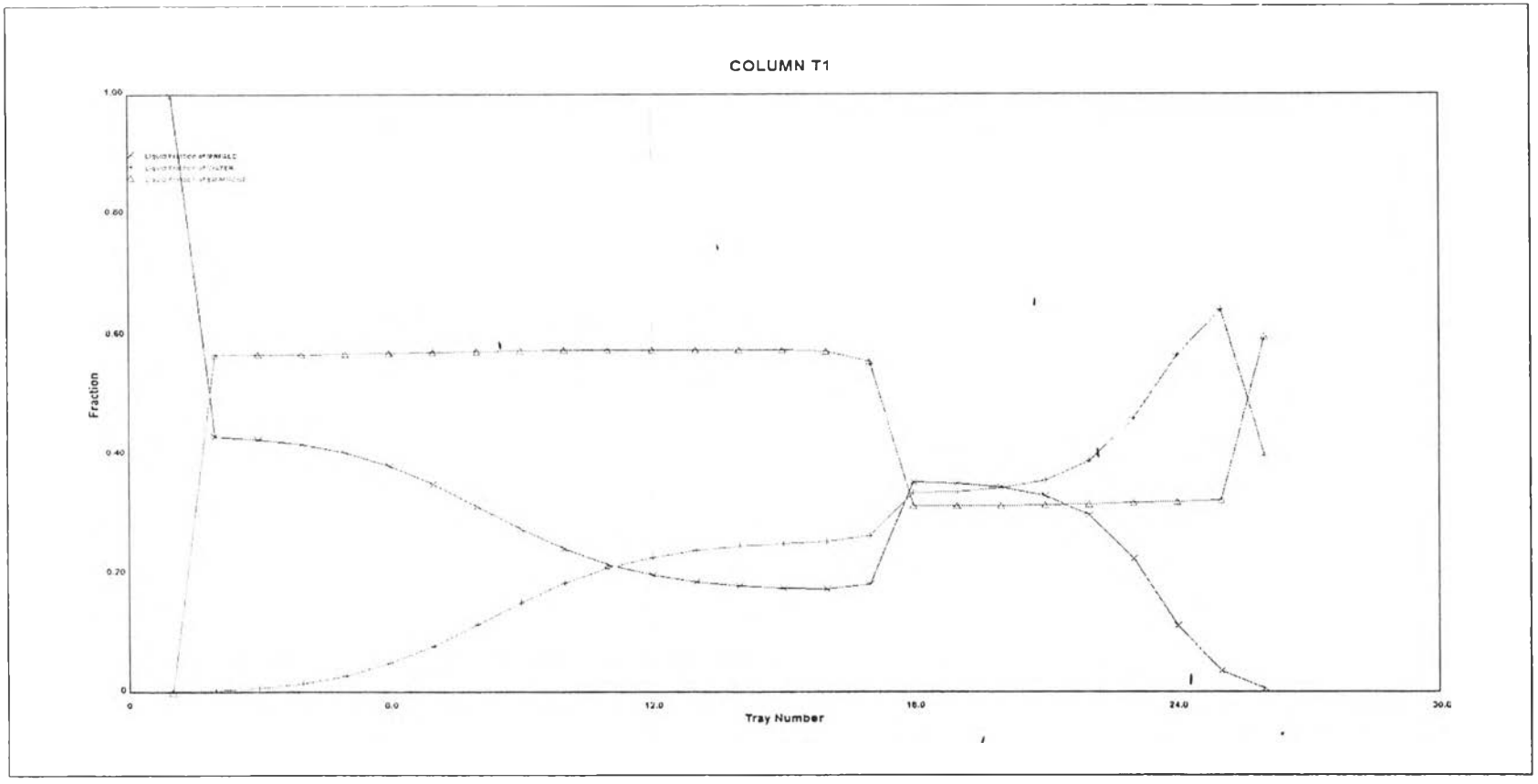

Figure D49 Overview of liquid fraction of the components in the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

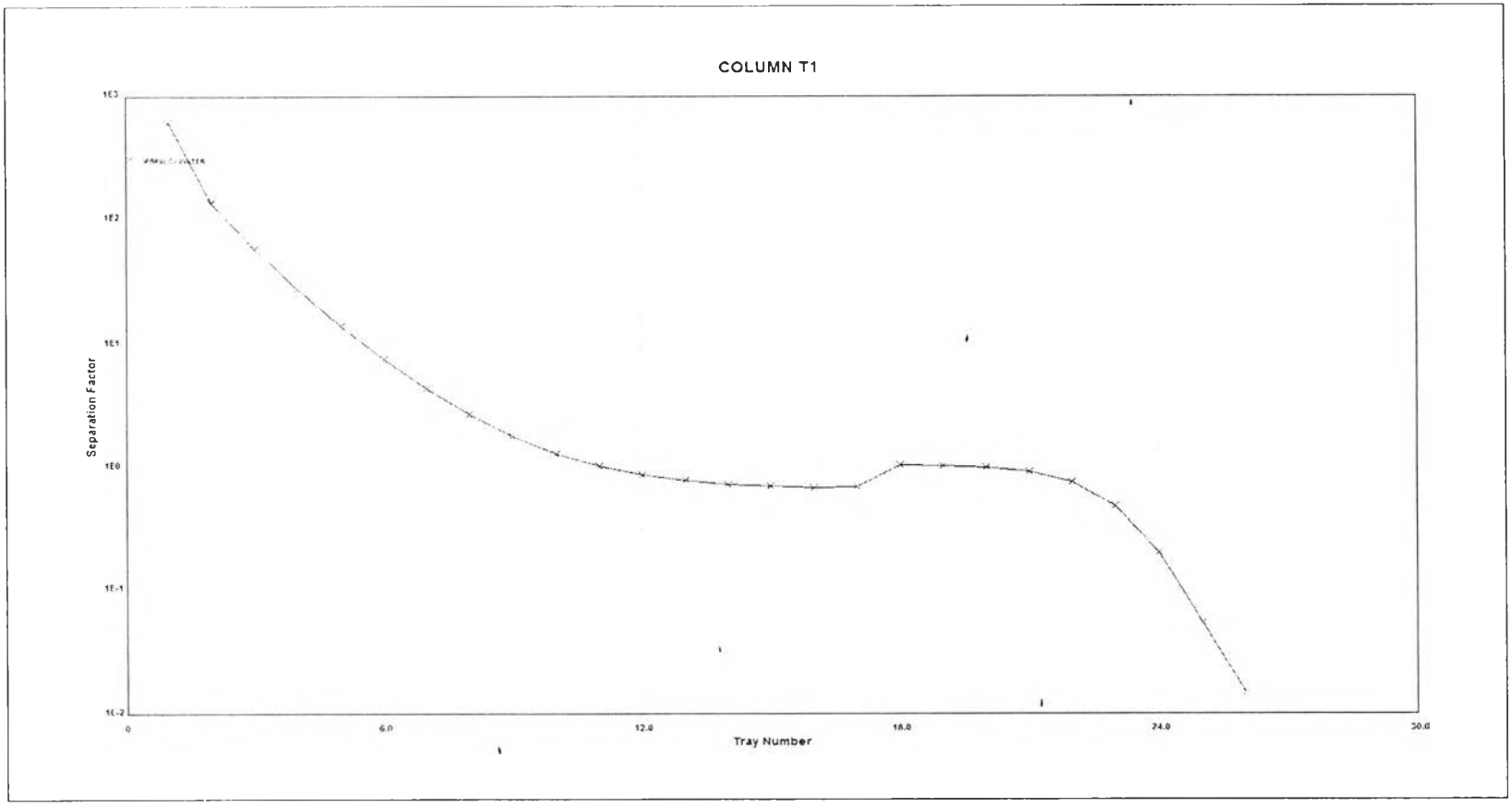

Figure D50 Separation factor in the extractive distillation process (column T1) using $[C_2mim][N(CN)_2]$ vs. tray number.

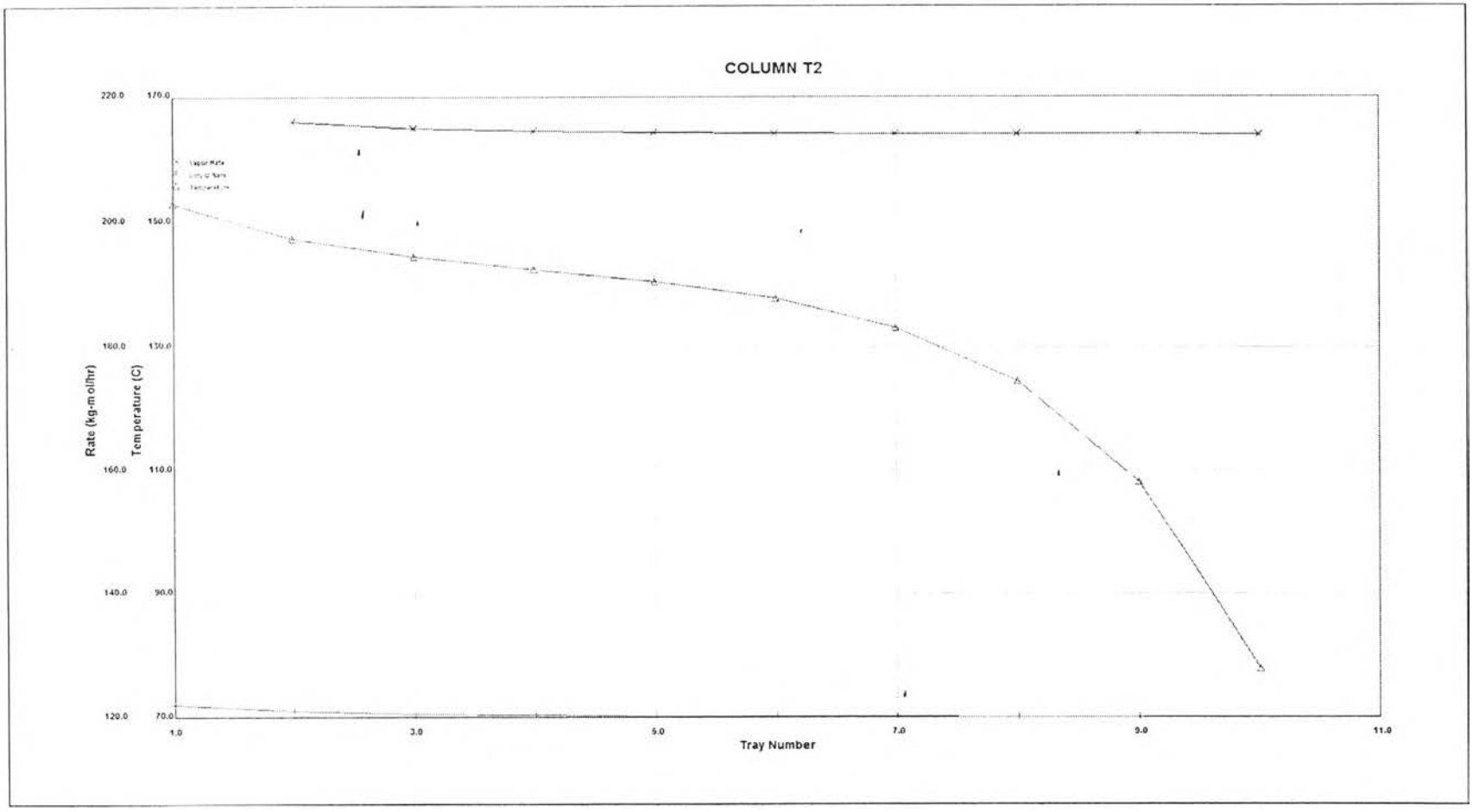

Figure D51 Overview of temperature and flowrate in the stripping column (column T2) using $[C_2mim][N(CN)_2]$ vs. tray number.

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Proceedings:

1. Kulajanpeng, K.; Suriyapraphadilok, U.; and Gani, R. (2014, April 22) A systematic screening of ionic liquids (ILs) as entrainers and design of IL-based separation processes. Proceedings of the 5th Research Symposium on Petrochemical and Materials Technology and the 20th PPC Symposium on Petroleum, Petrochemicals, and Polymers, Bangkok, Thailand.
2. Kulajanpeng, K.; Suriyapraphadilok, U.; and Gani, R. (2014, August 23-27) Ionic-liquid based separation of azeotropic mixtures. Proceeding of the 17th Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction PRES 2014, Prague, Czech Republic.