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APPENDICES

Appendix A Supplementary Data in Mixture Selection Step

- Azeotropic and close-boiling mixtures (Table A1)

Table A1 List of different problem mixtures from several literatures

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Water	100	Ethanol	78.4	-	-	Binary	Homogeneous	Aqueous system (Water + Alcohol)	95.5%	-
Water	100	Propanol	97.2	-	-	Binary	Homogeneous	Aqueous system (Water + Alcohol)	71.7%	-
Water	100	Isopropanol	82.5	-	-	Binary	Homogeneous	Aqueous system (Water + Alcohol)	87.9%	-
Water	100	Butanol	117.8	-	-	Binary	Heterogeneous	Aqueous system (Water + Alcohol)	55%	-
Water	100	Formic acid	100.8	-	-	Binary	Homogeneous	Aqueous system (Water + Organic Acid)	77.5%	-
Water	100	Acetic acid	118.1	-	-	Binary	Homogeneous	Aqueous system (Water + Organic Acid)	17.7%	-
Water	100	Butyric acid	163.5	-	-	Binary	Homogeneous	Aqueous system (Water + Organic Acid)	18.4%	-
Water	100	Nitric acid	86	-	-	Binary	Homogeneous	Aqueous system (Water + Mineral Acid)	68%	-

Table A1 Lists of different problem mixtures from several literatures (Continued)

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Water	100	Perchloric acid	110	-	-	Binary	Homogeneous	Aqueous system (Water + Mineral Acid)	71.6%	-
Water	100	Hydrofluoric acid	19.9	-	-	Binary	Homogeneous	Aqueous system (Water + Mineral Acid)	37%	-
Water	100	Sulfuric acid	290	-	-	Binary	Homogeneous	Aqueous system (Water + Mineral Acid)	98%	-
Water	100	Ethylene chloride	83.7	-	-	Binary	Homogeneous	Aqueous system (Water + alkyl halide)	91.8%	-
Water	100	Propylene chloride	96.8	-	-	Binary	Homogeneous	Aqueous system (Water + alkyl halide)	89.4%	-
Water	100	Ethyl acetate	77.1	-	-	Binary	Heterogeneous	Aqueous system (Water + ester)	91.9%	-
Water	100	Methyl acetate	57	-	-	Binary	Homogeneous	Aqueous system (Water + ester)	95%	-
Water	100	Benzene	80.2	-	-	Binary	Heterogeneous	Aqueous system (Water + aromatic)	91.1%	-
Water	100	Toluene	84.1	-	-	Binary	Heterogeneous	Aqueous system (Water + aromatic)	79.8%	-

Table A1 Lists of different problem mixtures from several literatures (Continued)

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Water	100	Cyclohexane	80.7	-	-	Binary	Heterogeneous	Aqueous system (Water + cyclic HC)	91.5%	-
Water	100	Acetonitrile	82	-	-	Binary	Homogeneous	Aqueous system (Water + Aliphatic HC)	83.7%	-
Ethanol	78.4	Pentane	36.2	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aliphatic HC)	95%	-
Ethanol	78.4	Hexane	68.9	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aliphatic HC)	79%	-
Ethanol	78.4	Heptane	98.5	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aliphatic HC)	51%	-
Ethanol	78.4	Octane	125.6	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aliphatic HC)	22%	-
Ethanol	78.4	Cyclohexane	80.7	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + cyclic HC)	69.5%	-
Ethanol	78.4	Benzene	80.2	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aromatic)	67.6%	-
Ethanol	78.4	Toluene	110.8	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aromatic)	32%	-

Table A1 Lists of different problem mixtures from several literatures (Continued)

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Ethanol	78.4	Ethyl acetate	77.1	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + ester)	69.2%	-
Ethanol	78.4	Methyl acetate	57	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + ester)	97%	-
Ethanol	78.4	Isopropyl acetate	88.4	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + ester)	47%	-
Ethanol	78.4	Ethylene chloride	83.7	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + alkyl halide)	63%	-
Ethanol	78.4	Propyl chloride	46.7	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + alkyl halide)	93%	-
Ethanol	78.4	Acetonitrile	82	-	-	Binary	Homogeneous	Non-aqueous system (Alcohol + Aliphatic HC)	43%	-
Ethanol	78.4	Thiophene	84.1	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + Aromatic)	55%	-
Benzene	80.1	Hexane	68.9	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + Aliphatic HC)	91%	-
Benzene	80.1	Heptane	98.5	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + Aliphatic HC)	99%	-

Table A1 Lists of different problem mixtures from several literatures (Continued)

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Benzene	80.1	Acetonitrile	73	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + Aliphatic HC)	34%	-
Benzene	80.1	Cyclohexane	81.4	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + cyclic HC)	45%	-
Toluene	110.8	Methanol	64.7	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + Alcohol)	72%	-
Toluene	110.8	Ethanol	78.4	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + Alcohol)	68%	-
Toluene	110.8	Acetic acid	118.5	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + organic acid)	28%	-
Toluene	110.8	Heptane	98.5	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + aliphatic HC)	Close-boiling	
Toluene	110.8	Cyclohexane	81	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + cyclic HC)	Close-boiling	
Toluene	110.8	Methylcyclohexane	101	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + cyclic HC)	Close-boiling	
Toluene	110.8	Pyridine	115.3	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + aromatic)	22%	-

Table A1 Lists of different problem mixtures from several literatures (Continued)

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Toluene	110.8	Ethylene glycol	197.4	-	-	Binary	Homogeneous	Non-aqueous system (Aromatic + aliphatic HC)	6%	-
Water	100	Ethanol	78.4	Ethyl acetate	77.1	Ternary	Homogeneous	Aqueous system (Water + alcohol +ester)	9%	83.2%
Water	100	Ethanol	78.4	Cyclohexane	80.8	Ternary	Homogeneous	Aqueous system (Water + alcohol + cyclic HC)	17%	76%
Water	100	Ethanol	78.4	Benzene	80.2	Ternary	Heterogeneous	Aqueous system (Water + alcohol + aromatic)	18.5%	74.1%
Water	100	Ethanol	78.4	Acetonitrile	82	Ternary	Homogeneous	Aqueous system (Water + alcohol + aliphatic HC)	55%	44%
Water	100	Ethanol	78.4	Toluene	110.6	Ternary	Heterogeneous	Aqueous system (Water + alcohol + aromatic)	37%	51%
Water	100	Ethanol	78.4	Hexane	69	Ternary	Heterogeneous	Aqueous system (Water + alcohol + aliphatic HC)	12%	85%
Water	100	Ethanol	78.4	Heptane	98.4	Ternary	Heterogeneous	Aqueous system (Water + alcohol + aliphatic HC)	33%	60.9%
Water	100	Propanol	97.2	Cyclohexane	80.8	Ternary	Homogeneous	Aqueous system (Water + alcohol + cyclic HC)	10%	81.5%

Table A1 Lists of different problem mixtures from several literatures (Continued)

Problem mixture						No. of components	Phase form	Solution system	Azeotrope	
1st comp	B.P. (°C)	2nd comp	B.P. (°C)	3rd comp	B.P. (°C)				%wt. 2nd	%wt. 3rd
Water	100	Propanol	97.2	Benzene	80.2	Ternary	Homogeneous	Aqueous system (Water + alcohol +aromatic)	9%	82.4%
Water	100	Isopropanol	82.5	Cyclohexane	80.8	Ternary	Homogeneous	Aqueous system (Water + alcohol + cyclic HC)	21.5%	71%
Water	100	Isopropanol	82.5	Benzene	80.2	Ternary	Heterogeneous	Aqueous system (Water + alcohol +aromatic)	19.8%	72%
Water	100	Benzene	80.1	Acetonitrile	82	Ternary	Homogeneous	Aqueous system (Water + aromatic + aliphatic HC)	68.5%	23.3%

Appendix B Supplementary Data in IL Pre-Selection Step

- Screening graph (Table B1 and Figure B1-B30)
- Feasible IL candidates (Table B2-B6)

Table B1 List of the feasible and selected target solutes with the number of figures

Case study	Feasible target solutes	No. Figure	Selected target solute
Water + Ethanol	Ethanol	B1,B2,B3	Water
	Water	B4,B5,B6	
Ethanol + Hexane	Hexane	B7,B8,B9	Ethanol
	Ethanol	B10,B11,B12	
Benzene + Hexane	Hexane	B13,B14,B15	Benzene
	Benzene	B16,B17,B18	
Toluene + MCH	MCH	B19,B20,B21	Toluene
	Toluene	B22,B23,B24	
EB + PX	PX	B25,B26,B27	EB
	EB	B28,B29,B30	

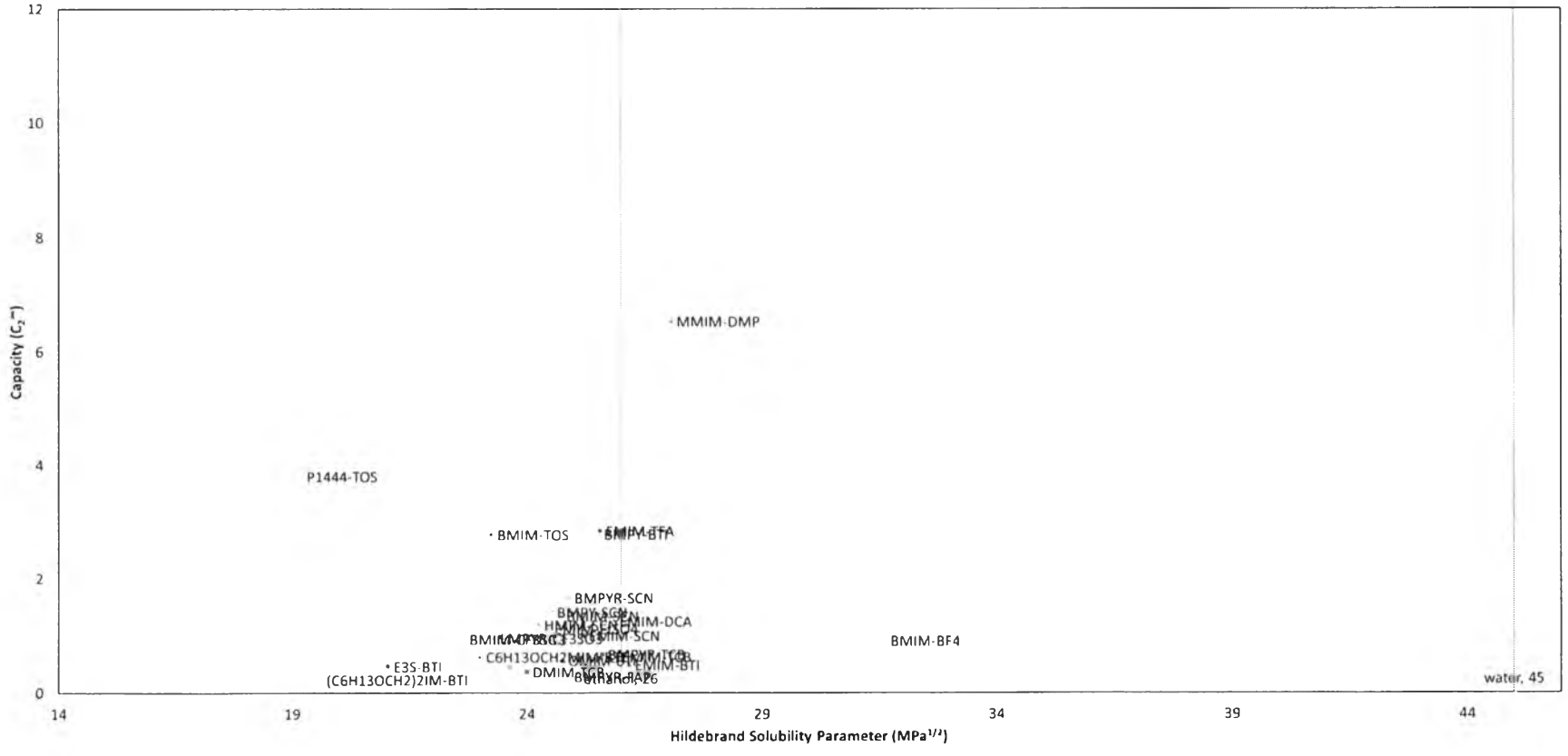

Figure B1 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^∞) of ILs (ethanol as target solute) (water + ethanol mixture).

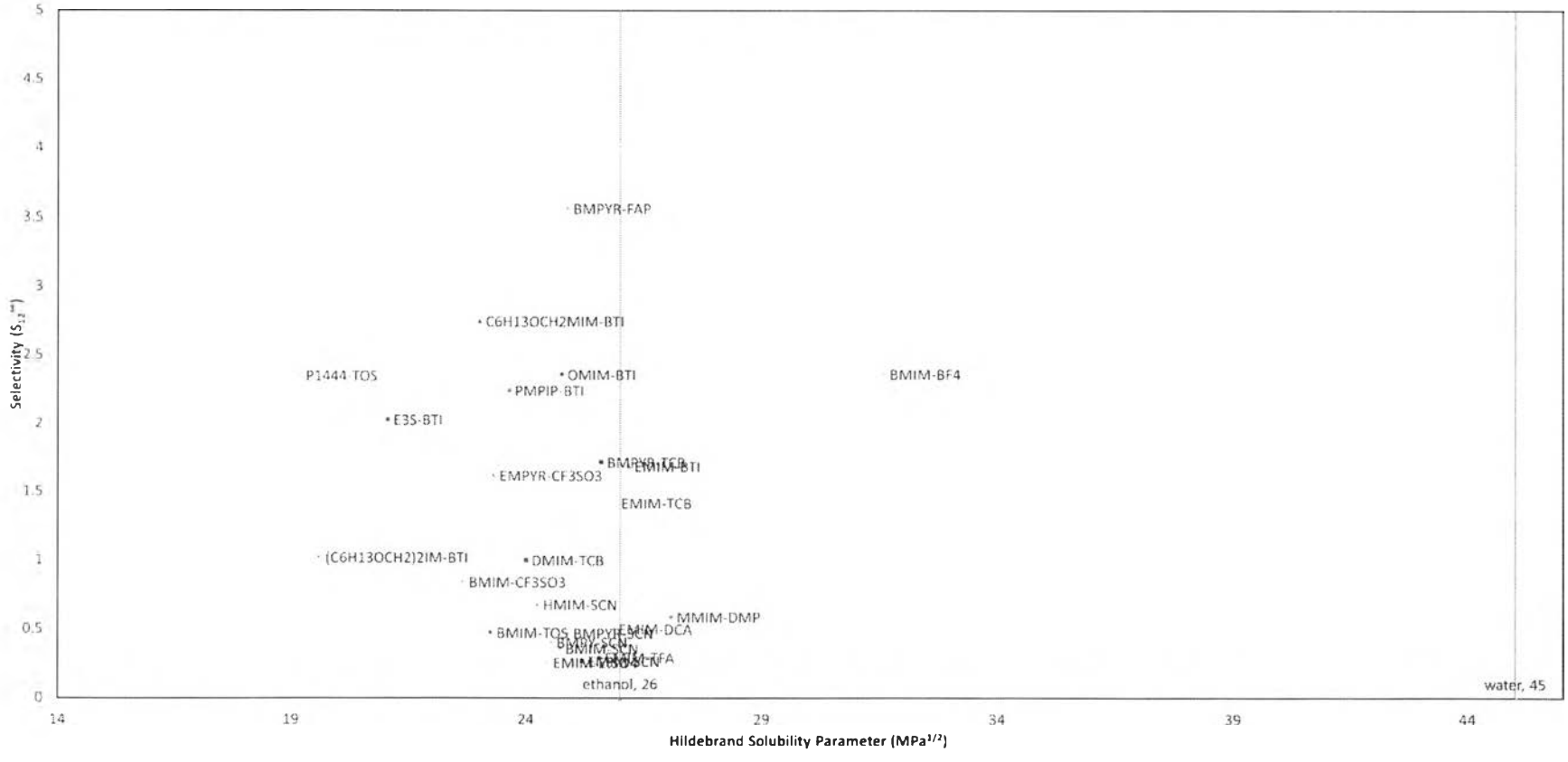

Figure B2 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (ethanol as target solute) (water + ethanol mixture).

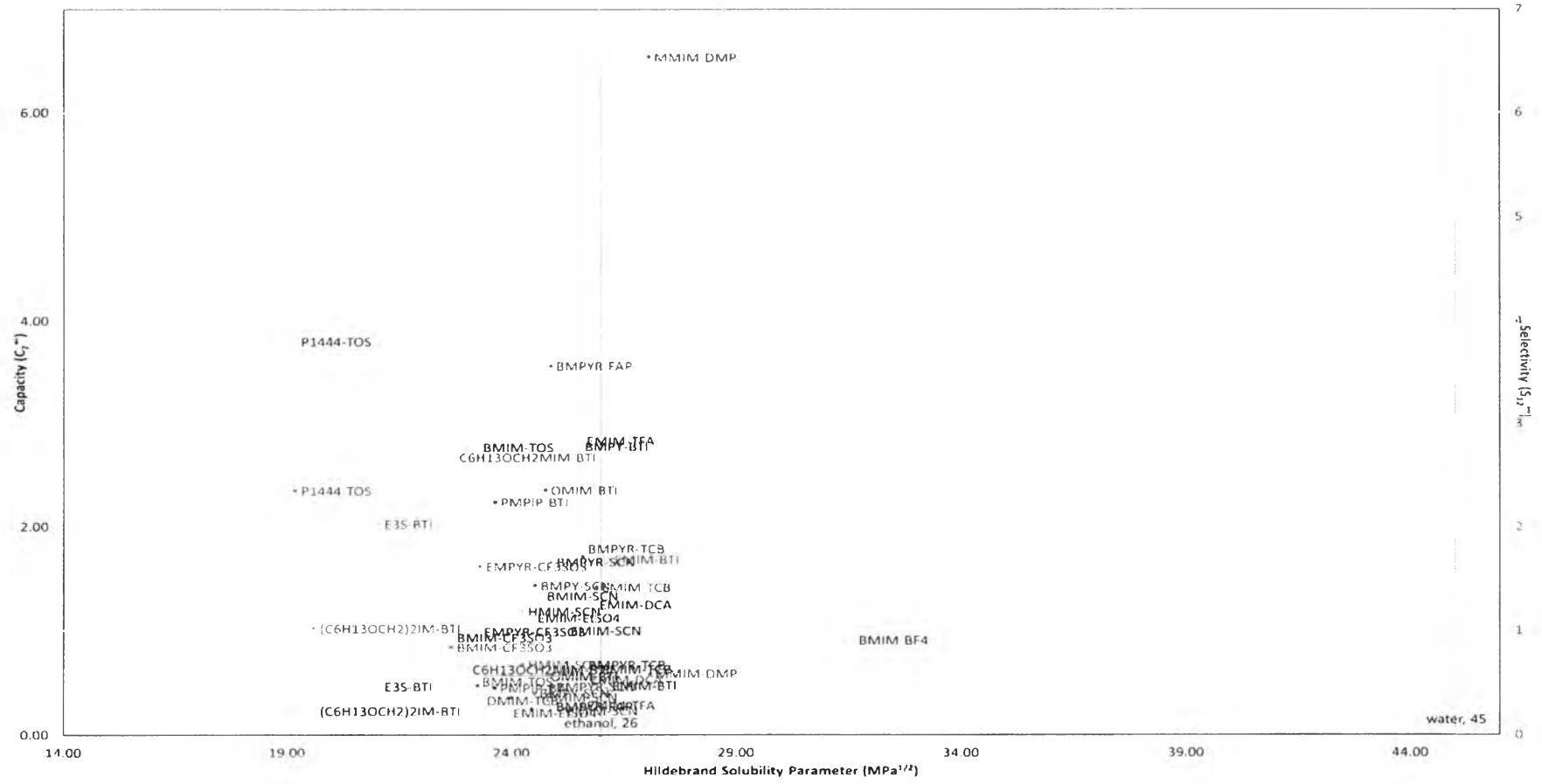

Figure B3 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^{∞}) of ILs (primary *y-axis*) and Selectivity (S_{12}^{∞}) of ILs (secondary *y-axis*) of the water + ethanol mixture. Ethanol is the target solute.

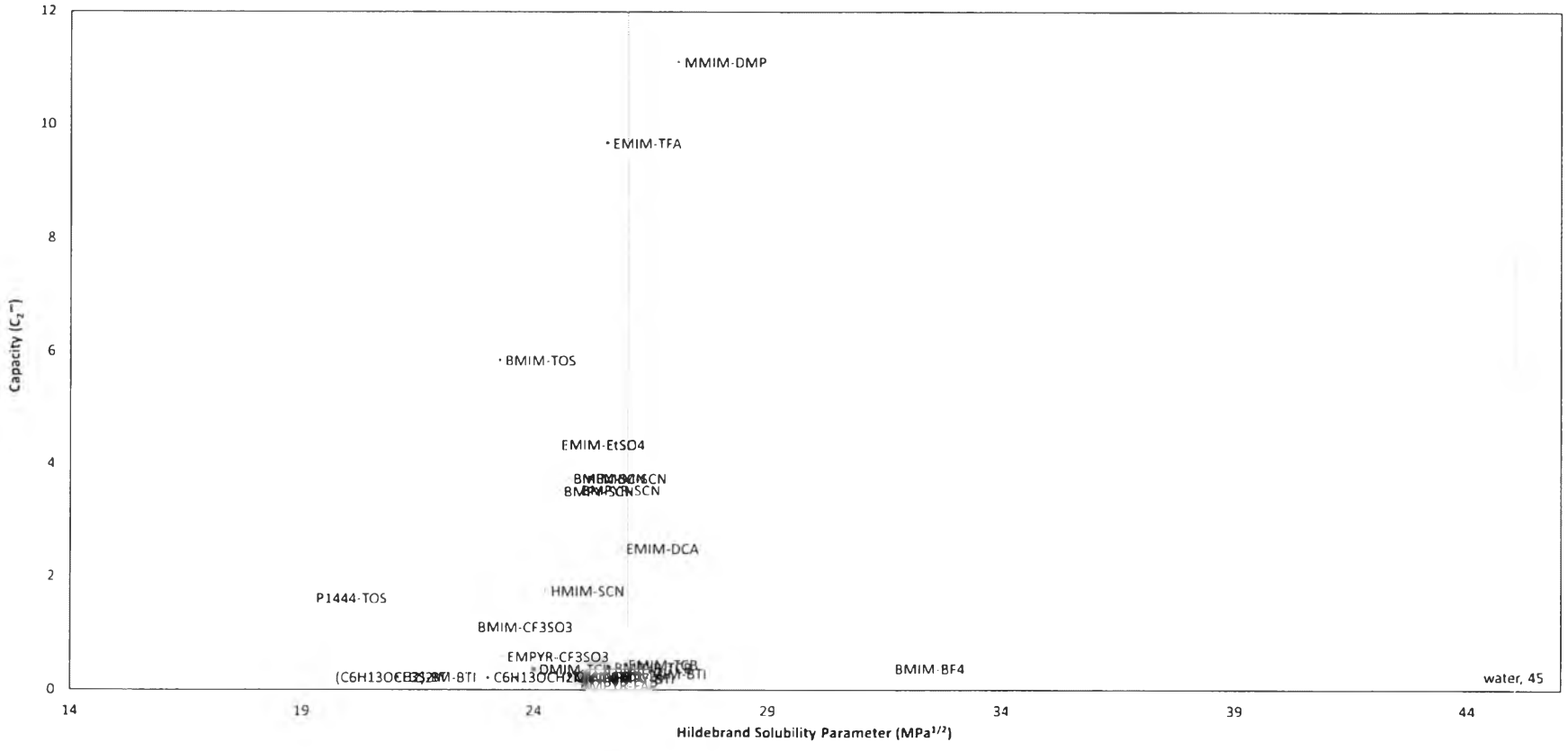

Figure B4 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^{∞}) of ILs (water as target solute) (water + ethanol mixture).

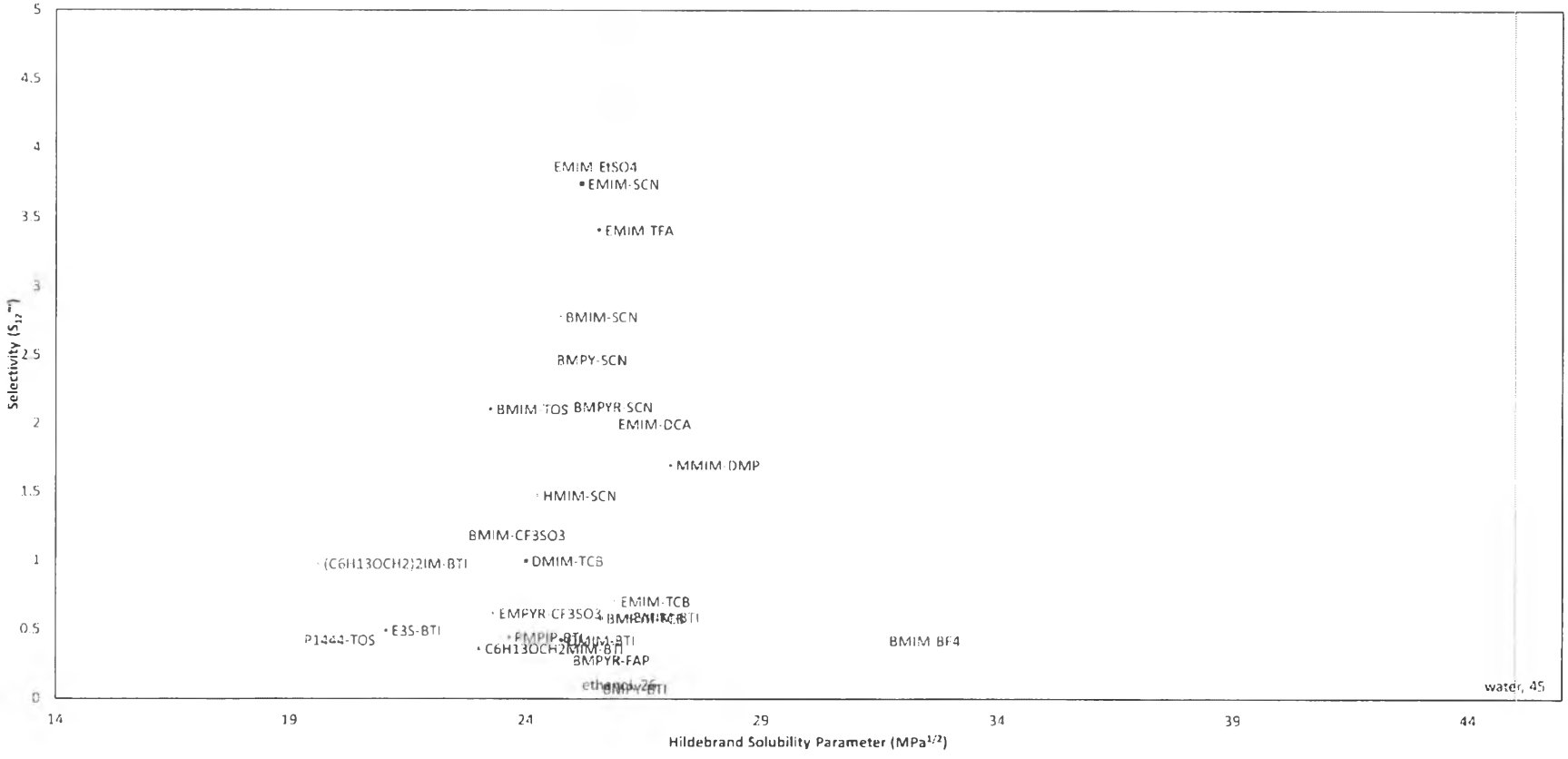

Figure B5 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (ethanol as target solute) (water + ethanol mixture).

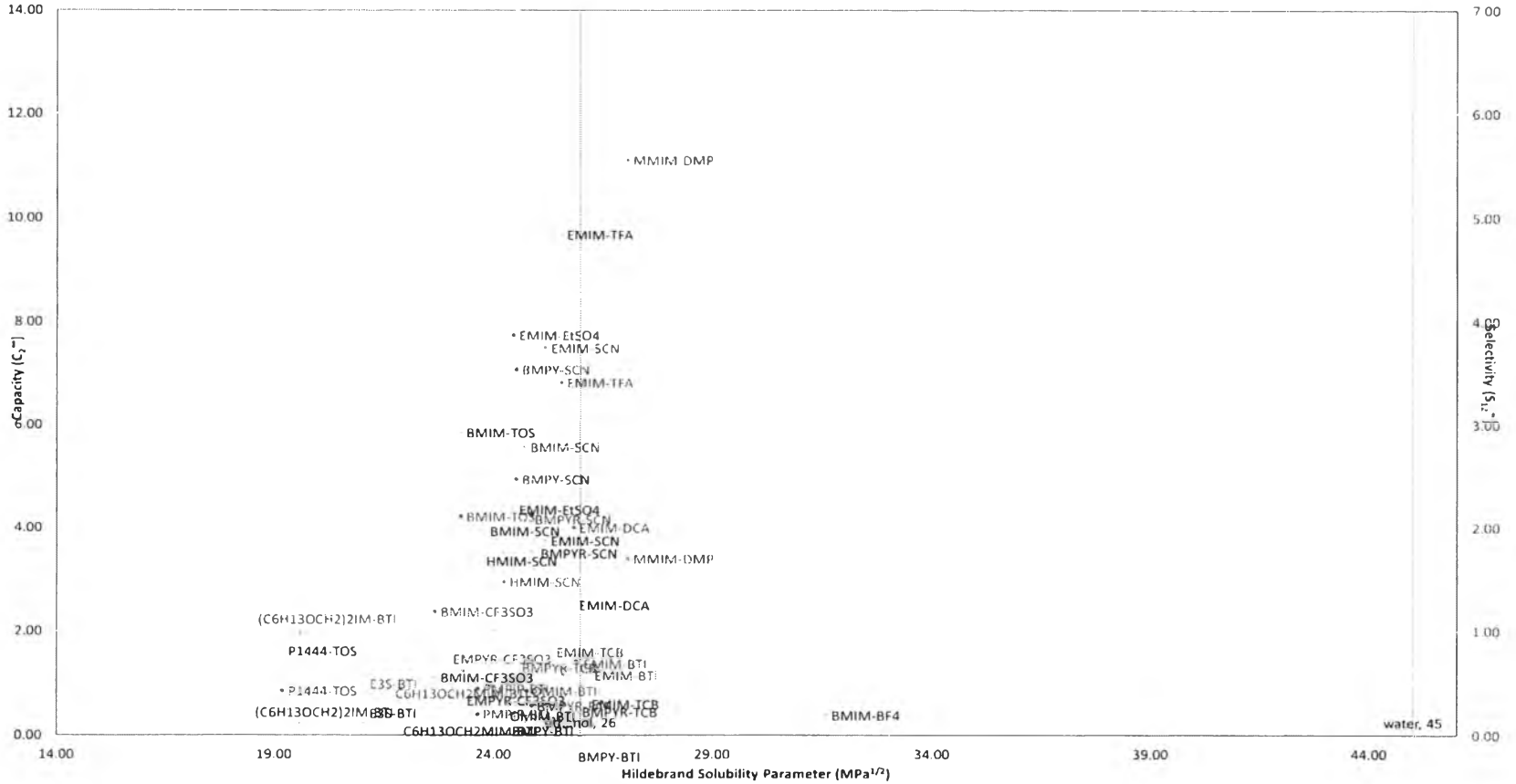

Figure B6 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^{∞}) of ILs (primary *y-axis*) and Selectivity (S_{12}^{∞}) of ILs (secondary *y-axis*) of the water + ethanol mixture. Water is the target solute.

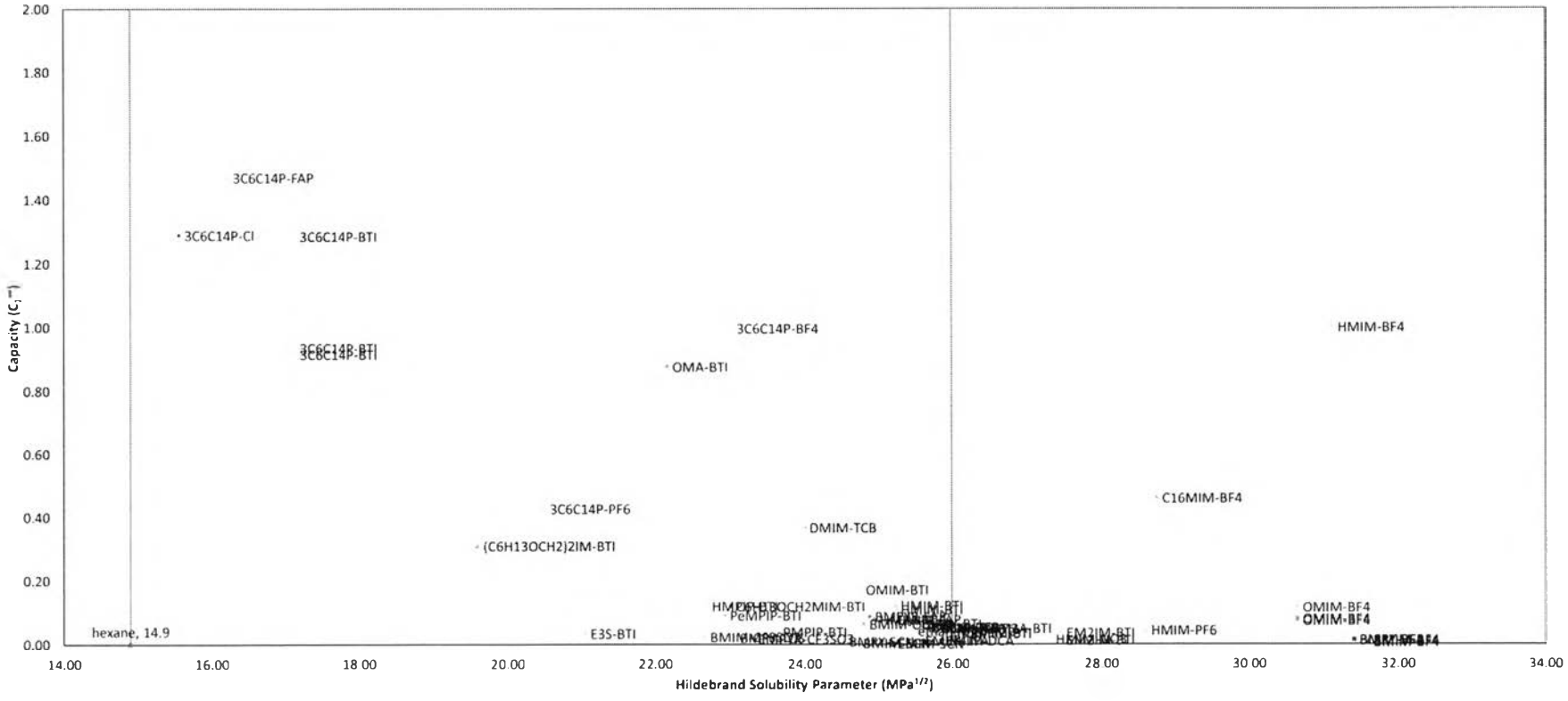

Figure B7 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^{∞}) of ILs (hexane as target solute) (ethanol + hexane mixture).

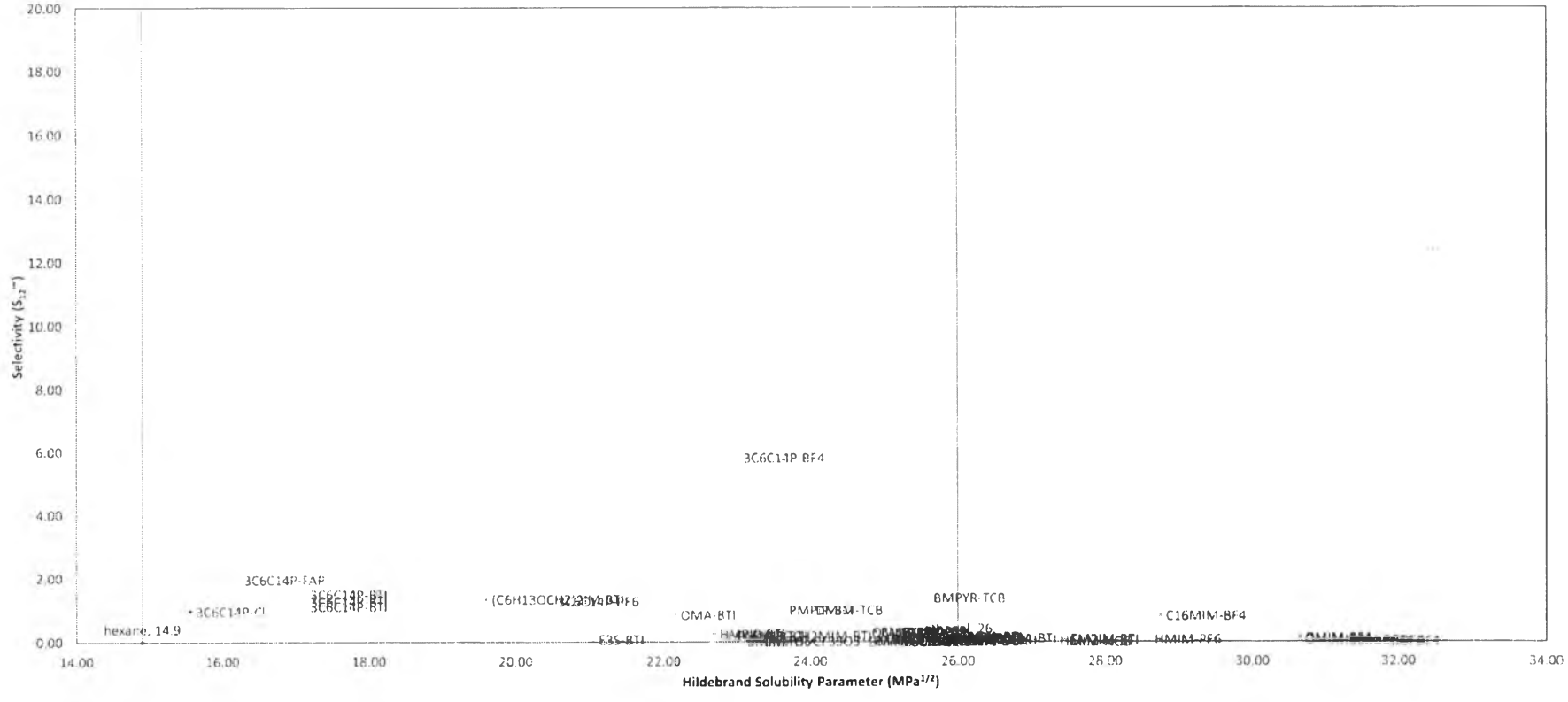

Figure B8 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (hexane as target solute) (ethanol + hexane mixture).

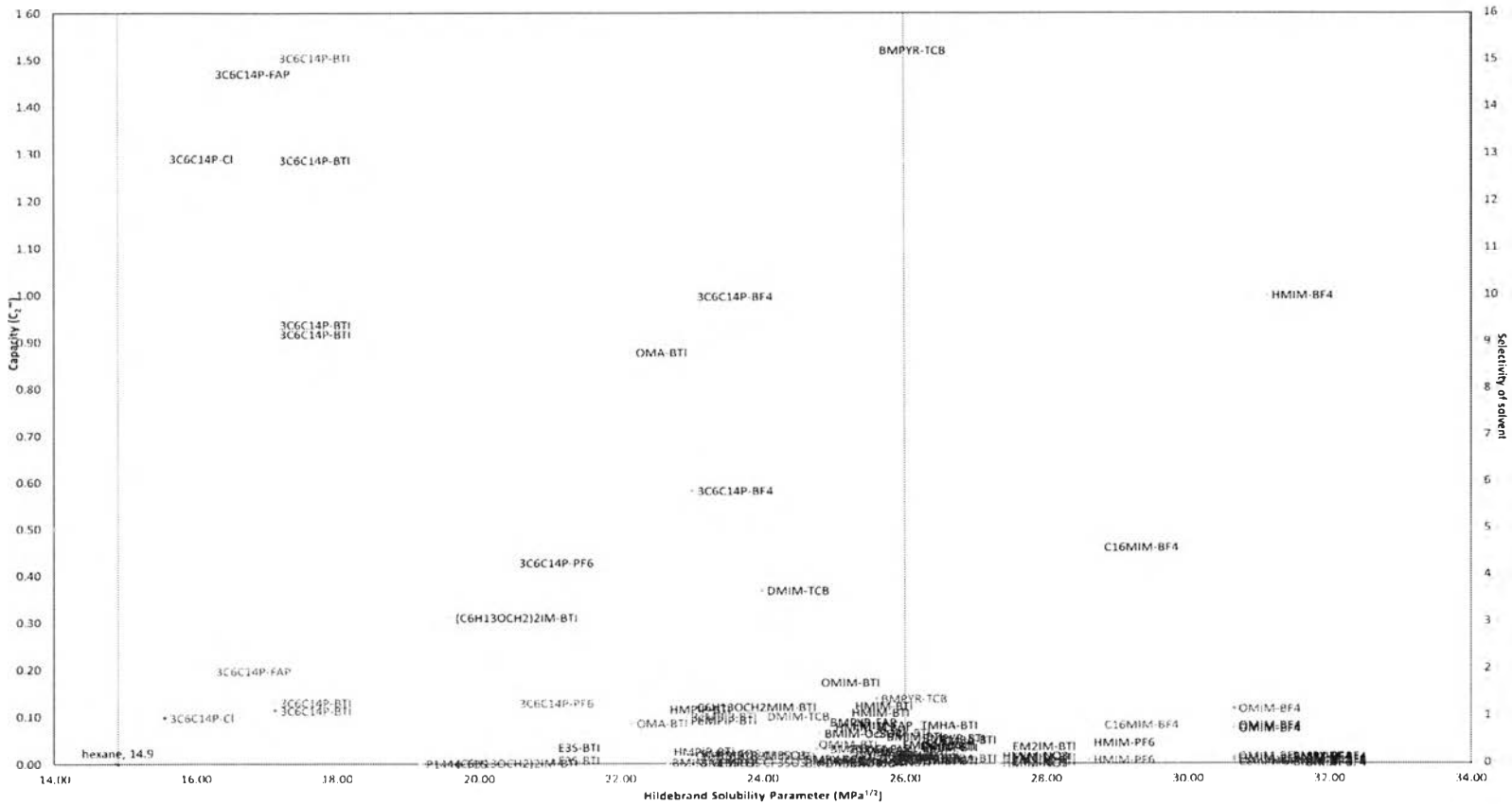

Figure B9 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the ethanol + hexane mixture. Hexane is the target solute.

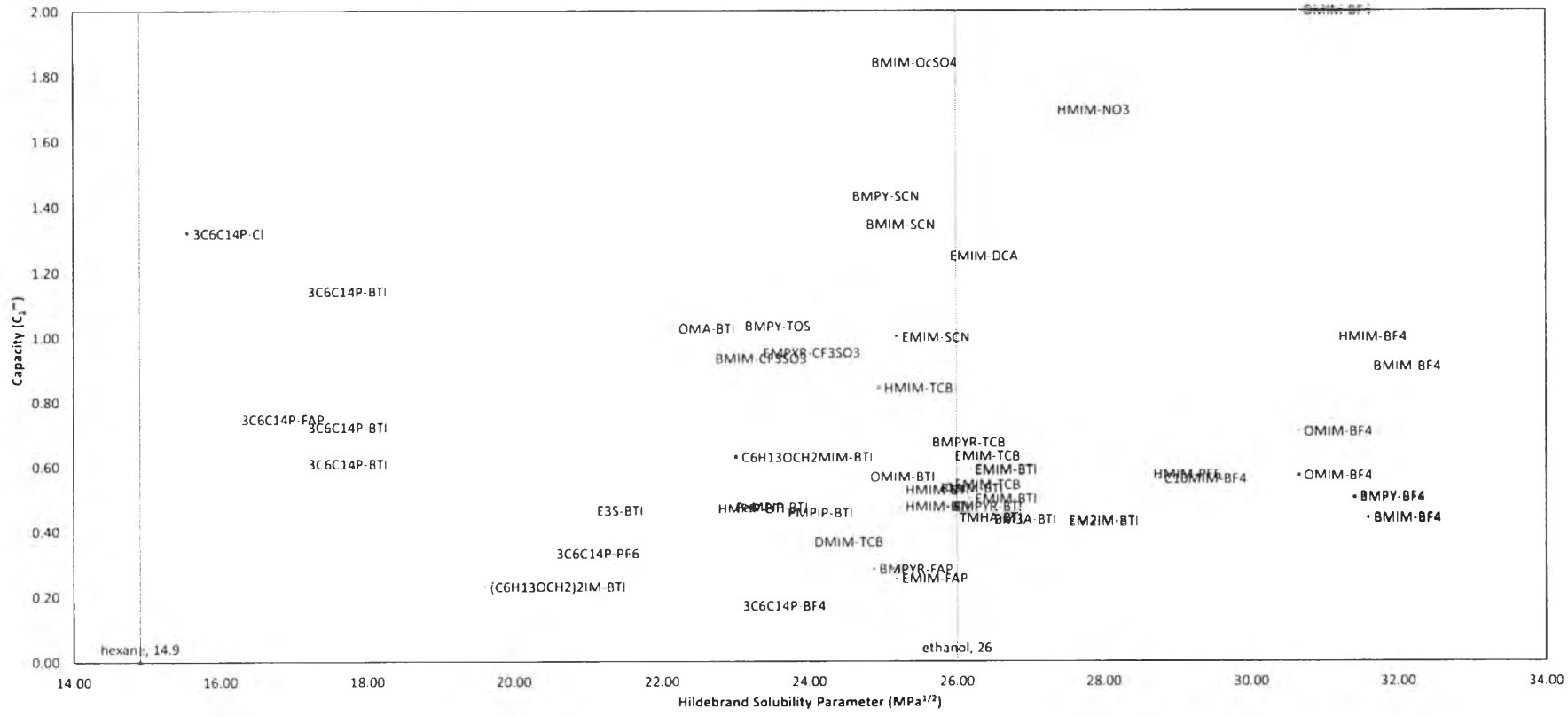

Figure B10 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^{∞}) of ILs (ethanol as target solute) (ethanol + hexane mixture).

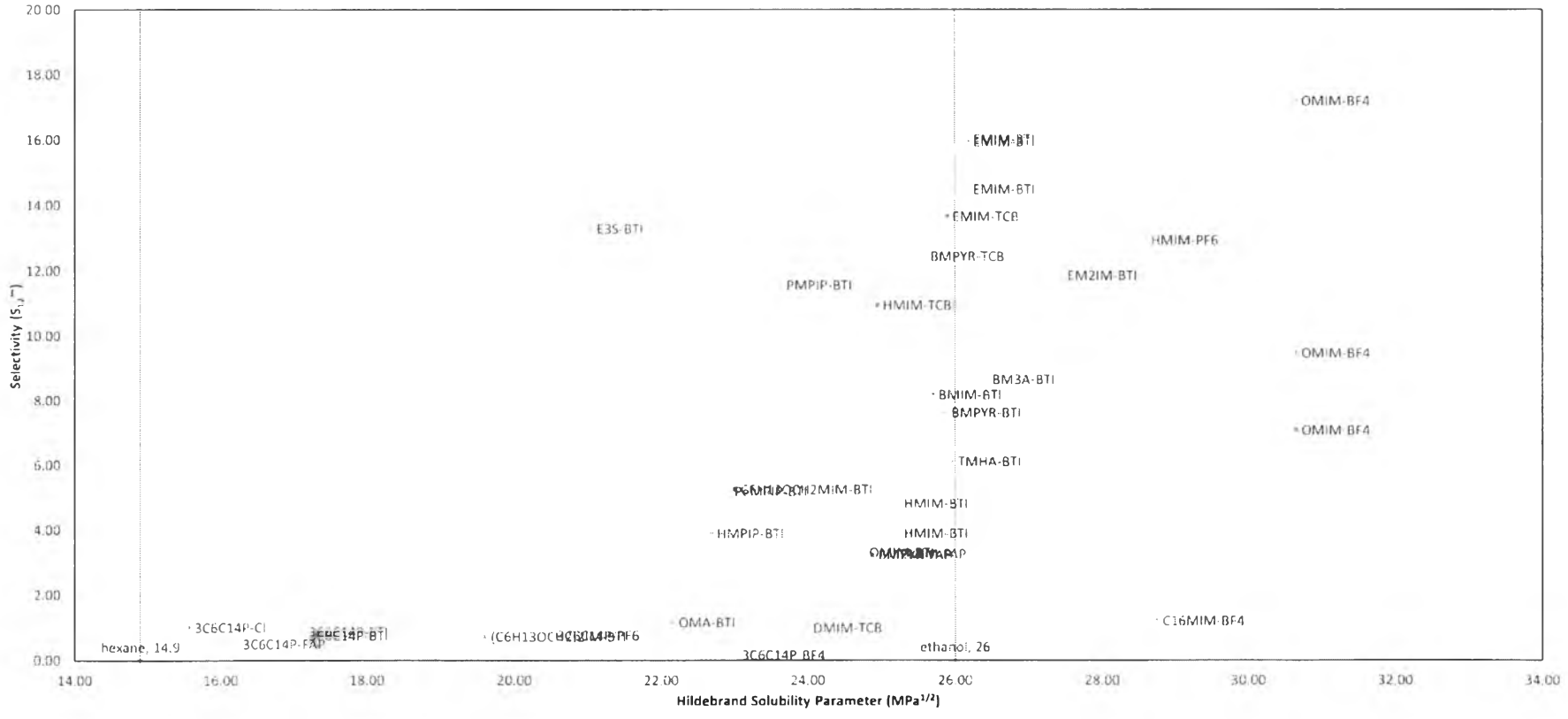

Figure B11 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (ethanol as target solute) (ethanol + hexane mixture).

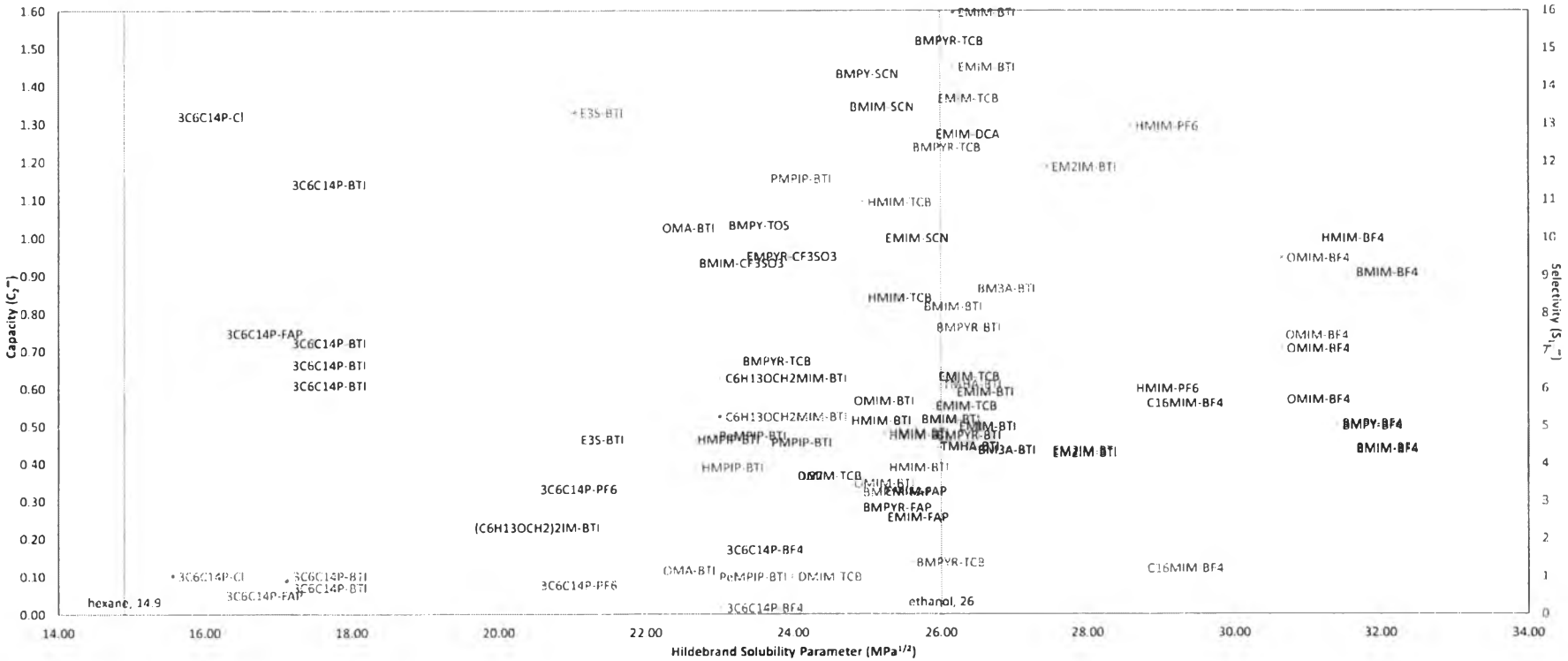

Figure B12 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the ethanol + hexane mixture. Ethanol is the target solute.

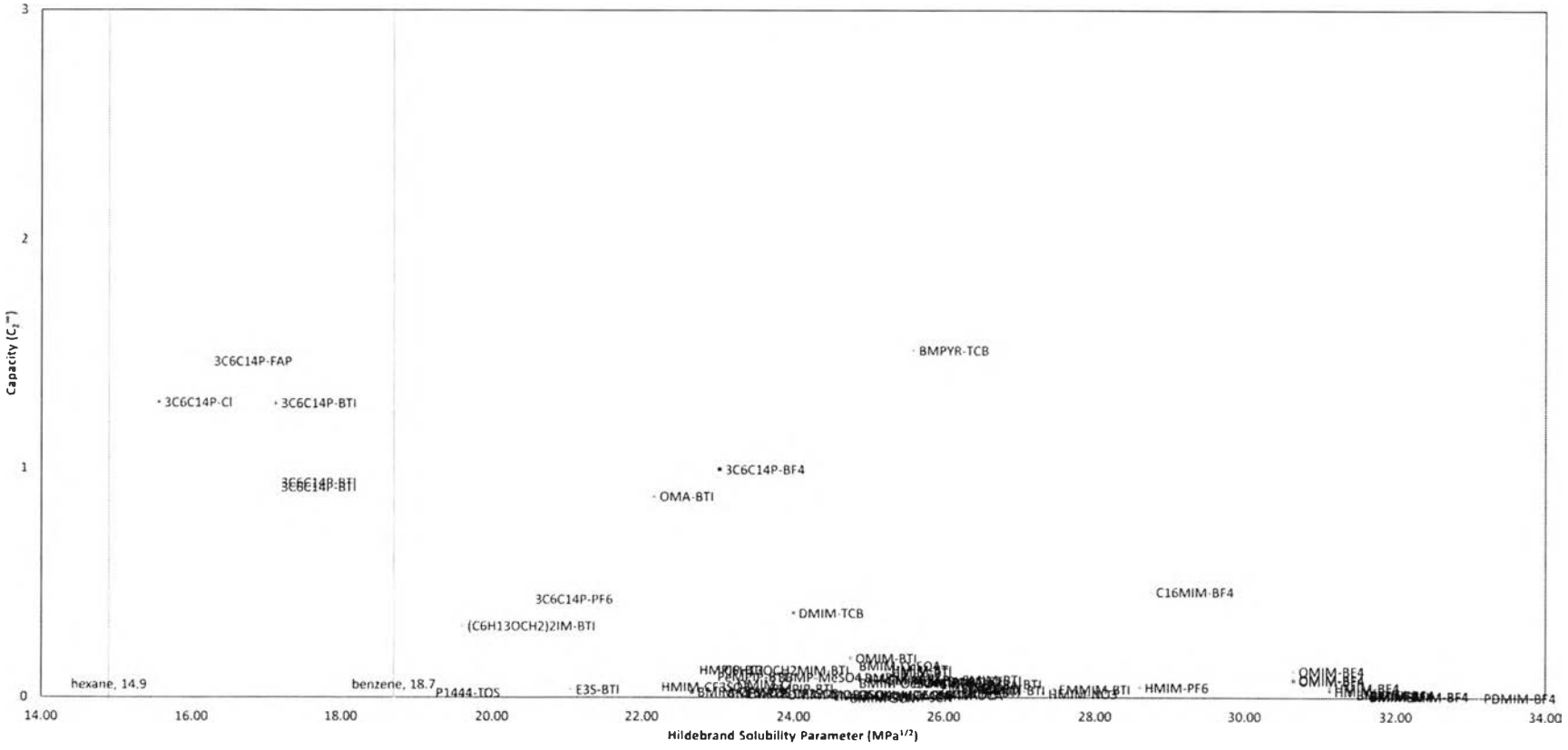

Figure B13 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^∞) of ILs (hexane as target solute) (benzene + hexane mixture).

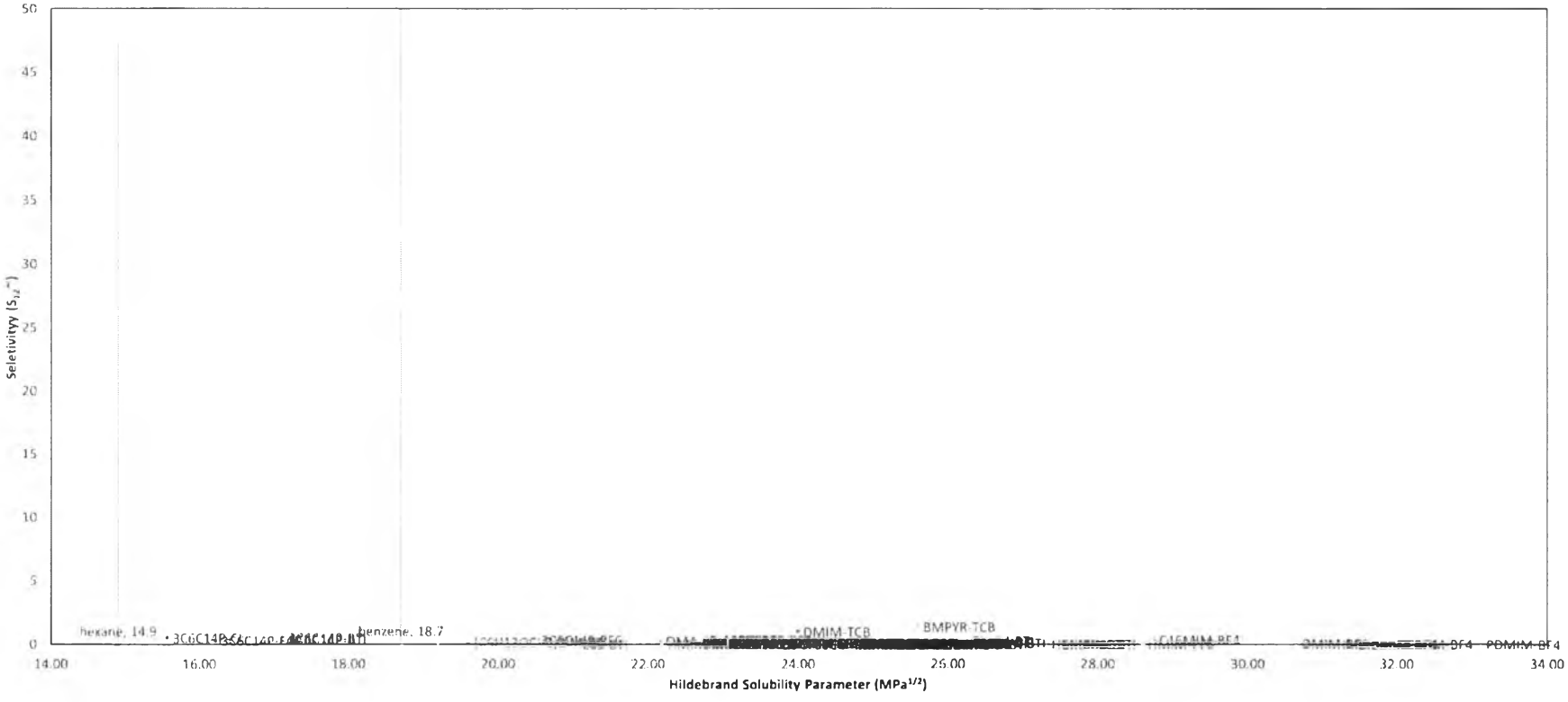

Figure B14 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (hexane as target solute) (benzene + hexane mixture).

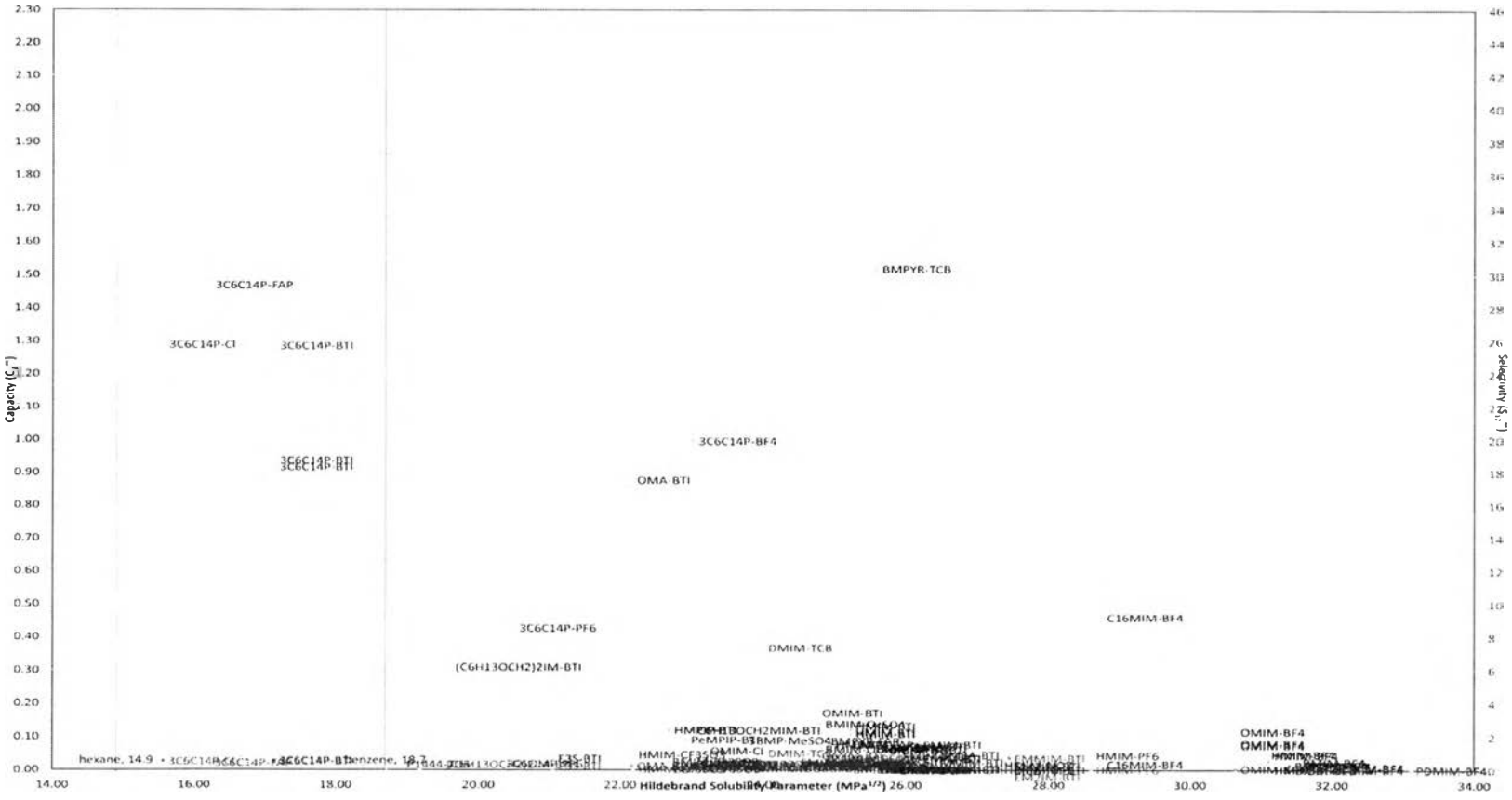

Figure B15 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^{∞}) of ILs (primary *y-axis*) and Selectivity (S_{12}^{∞}) of ILs (secondary *y-axis*) of the benzene + hexane mixture. Hexane is the target solute.

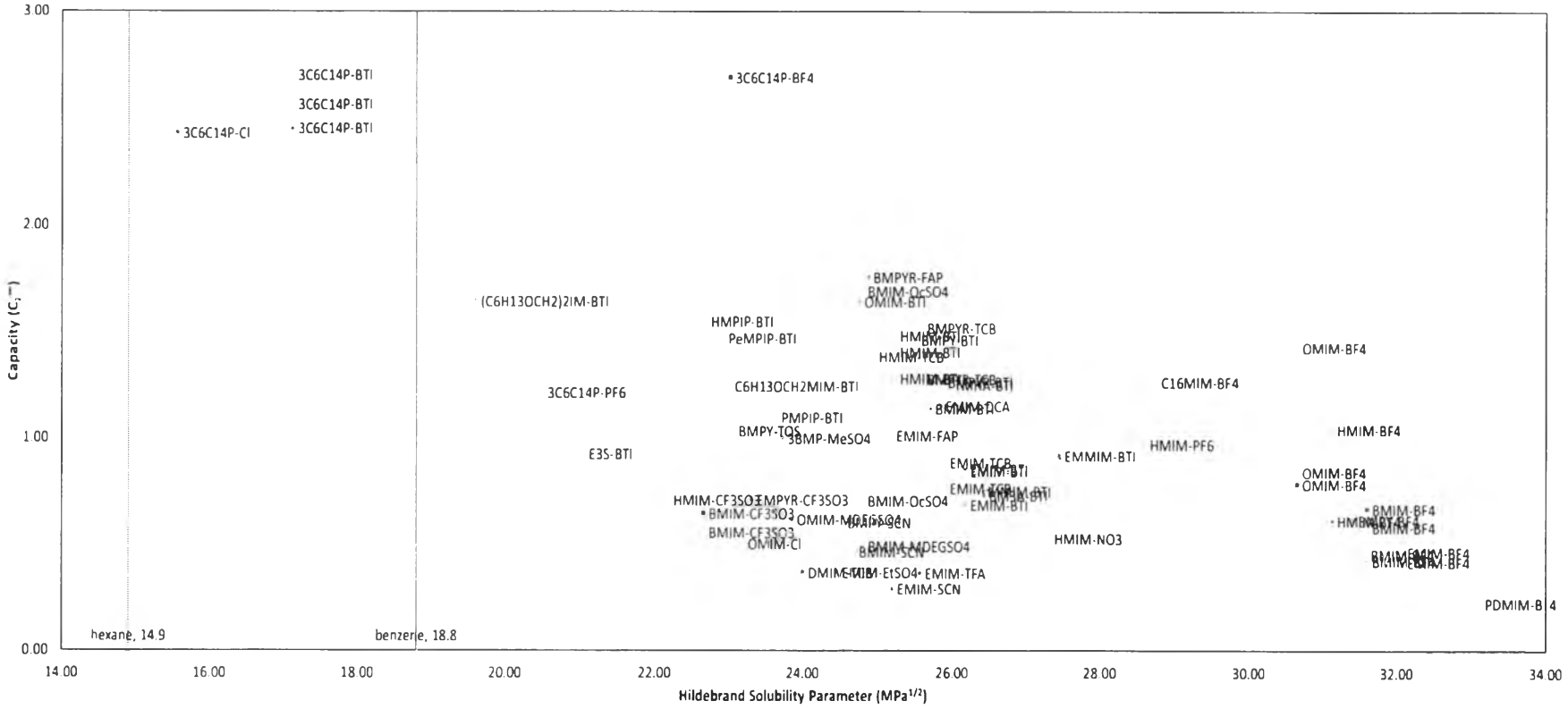

Figure B16 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^{∞}) of ILs (benzene as target solute) (benzene + hexane mixture).

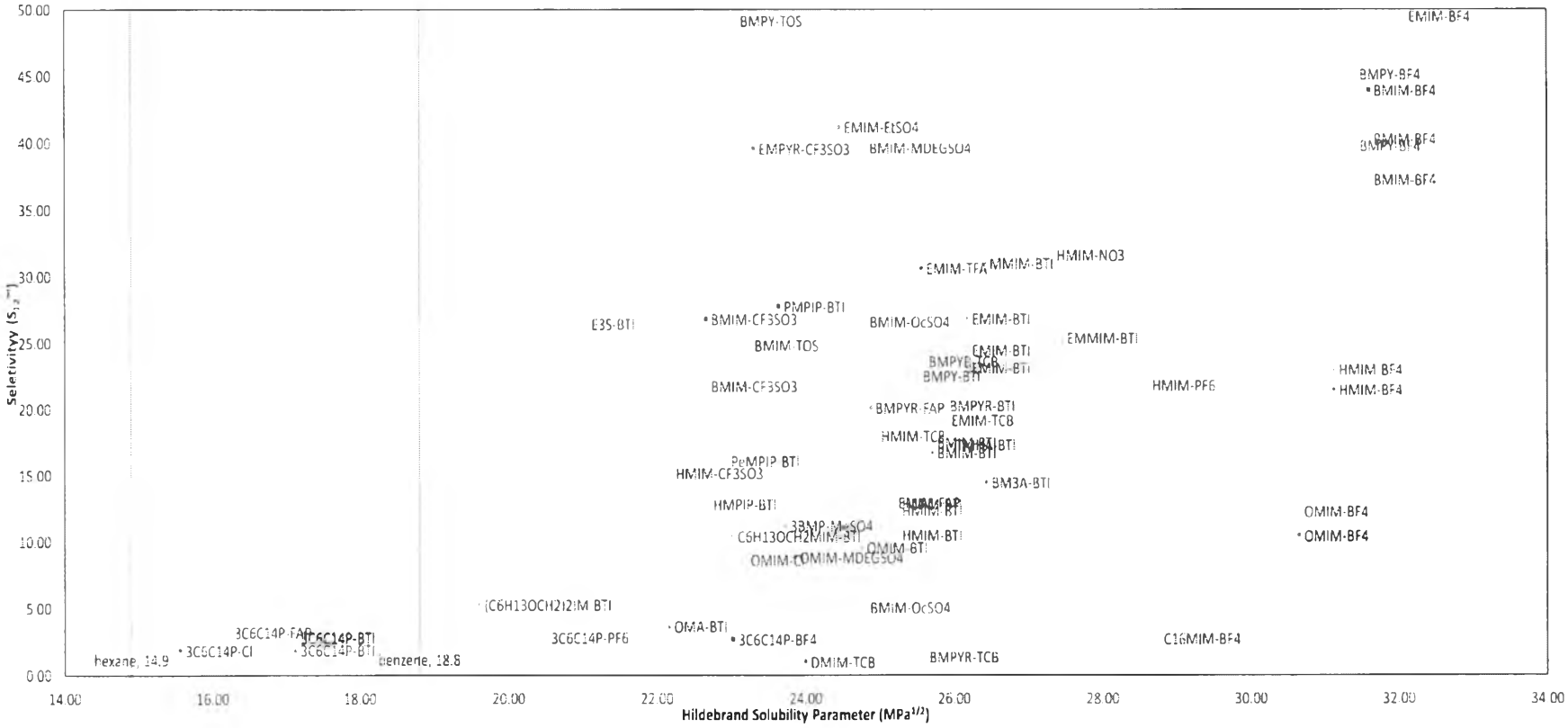

Figure B17 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (benzene as target solute) (benzene + hexane mixture).

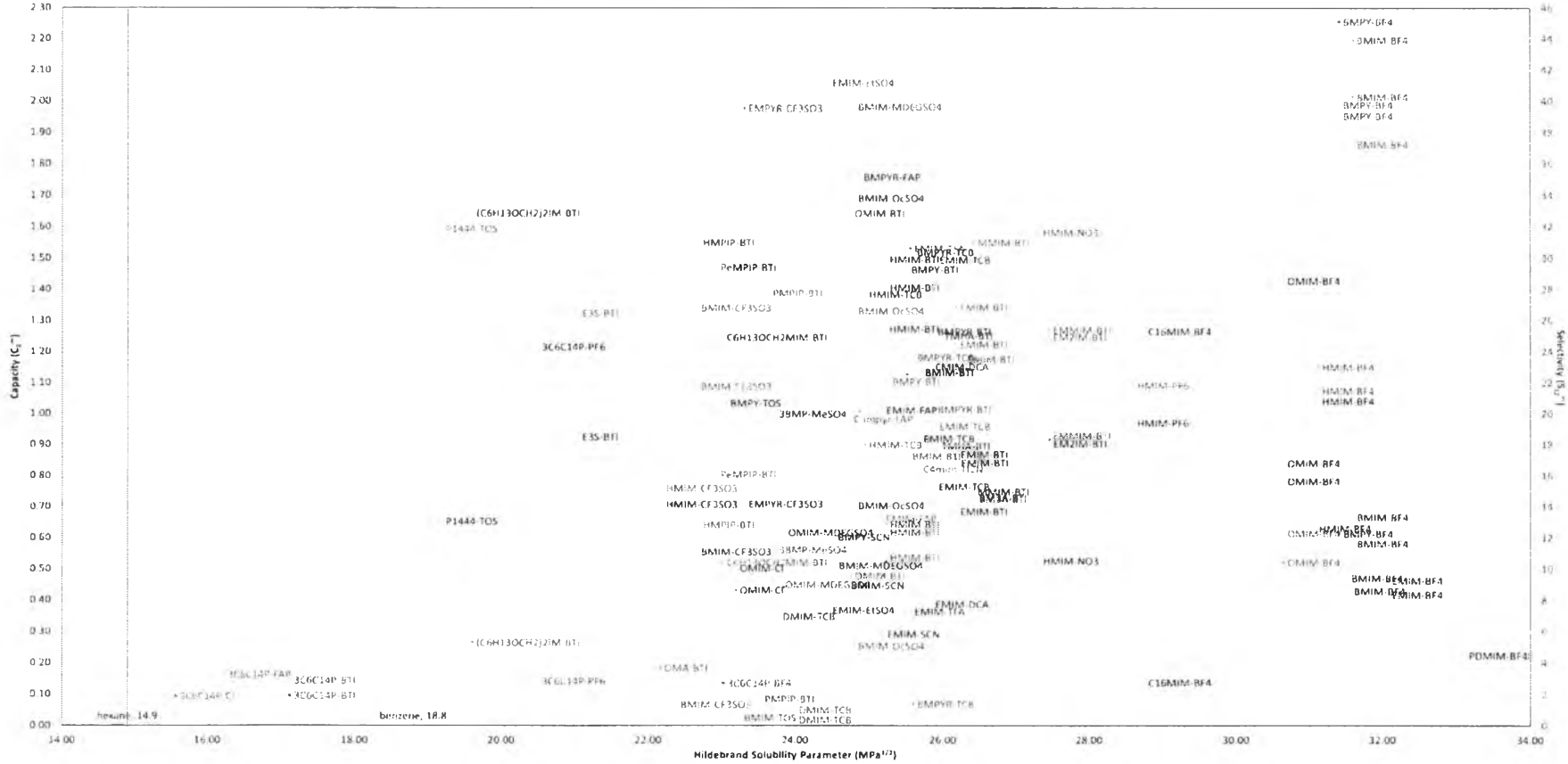

Figure B18 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the benzene + hexane mixture. Benzene is the target solute.

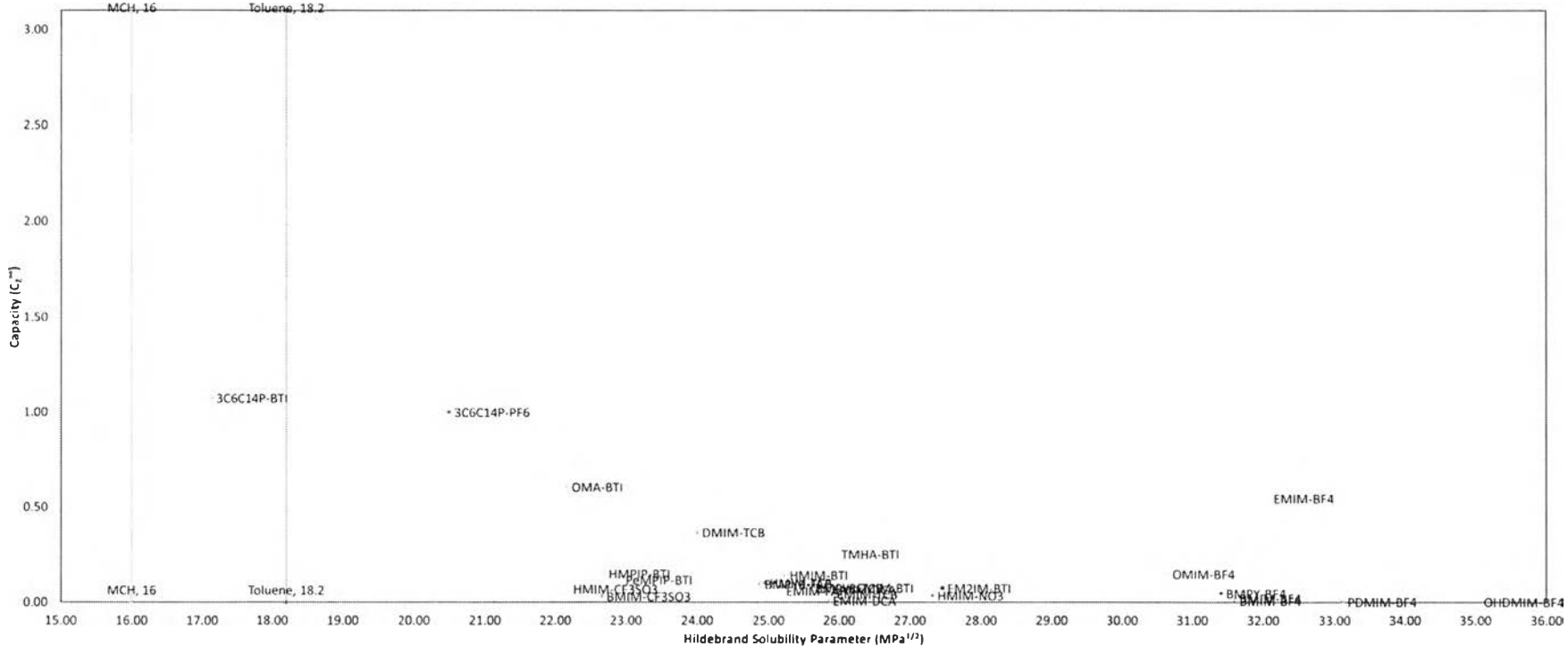

Figure B19 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^∞) of ILs (MCH as target solute) (Toluene + MCH mixture).

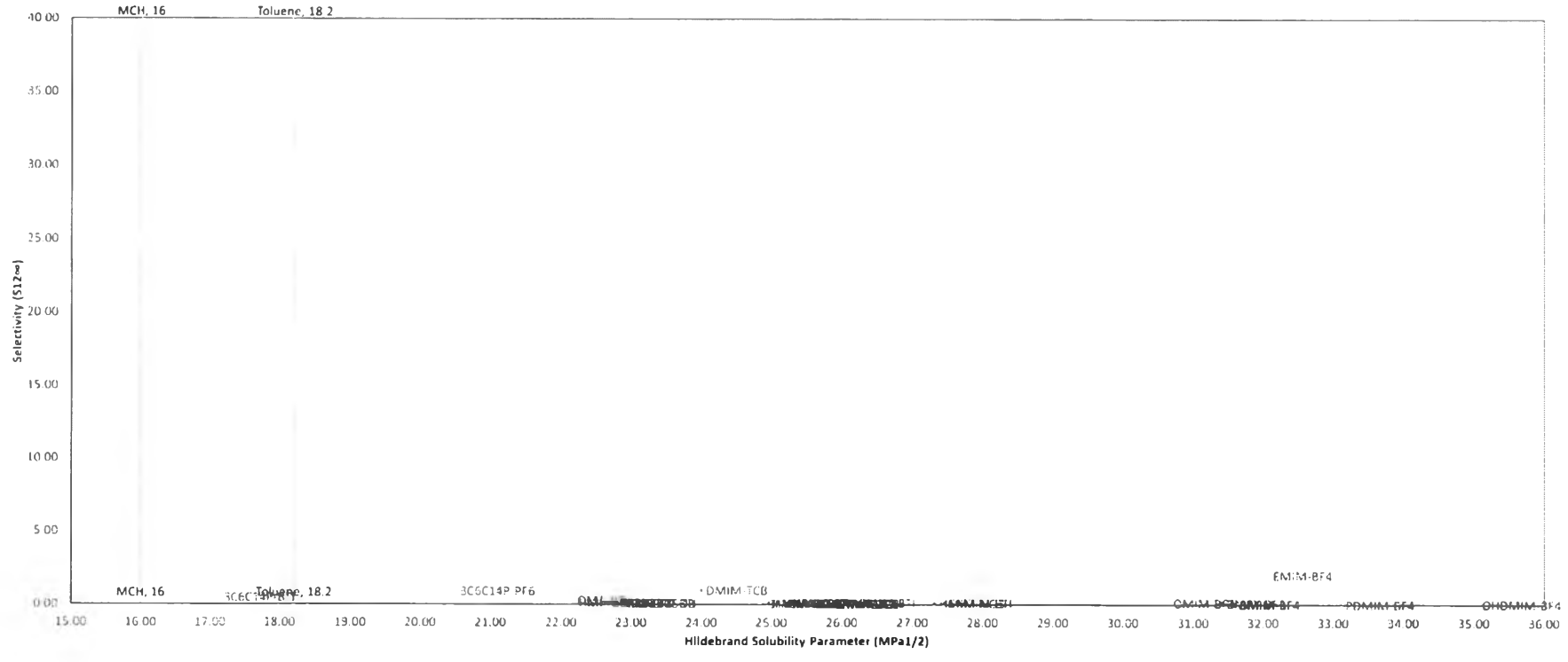

Figure B20 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (MCH as target solute) (Toluene + MCH mixture).

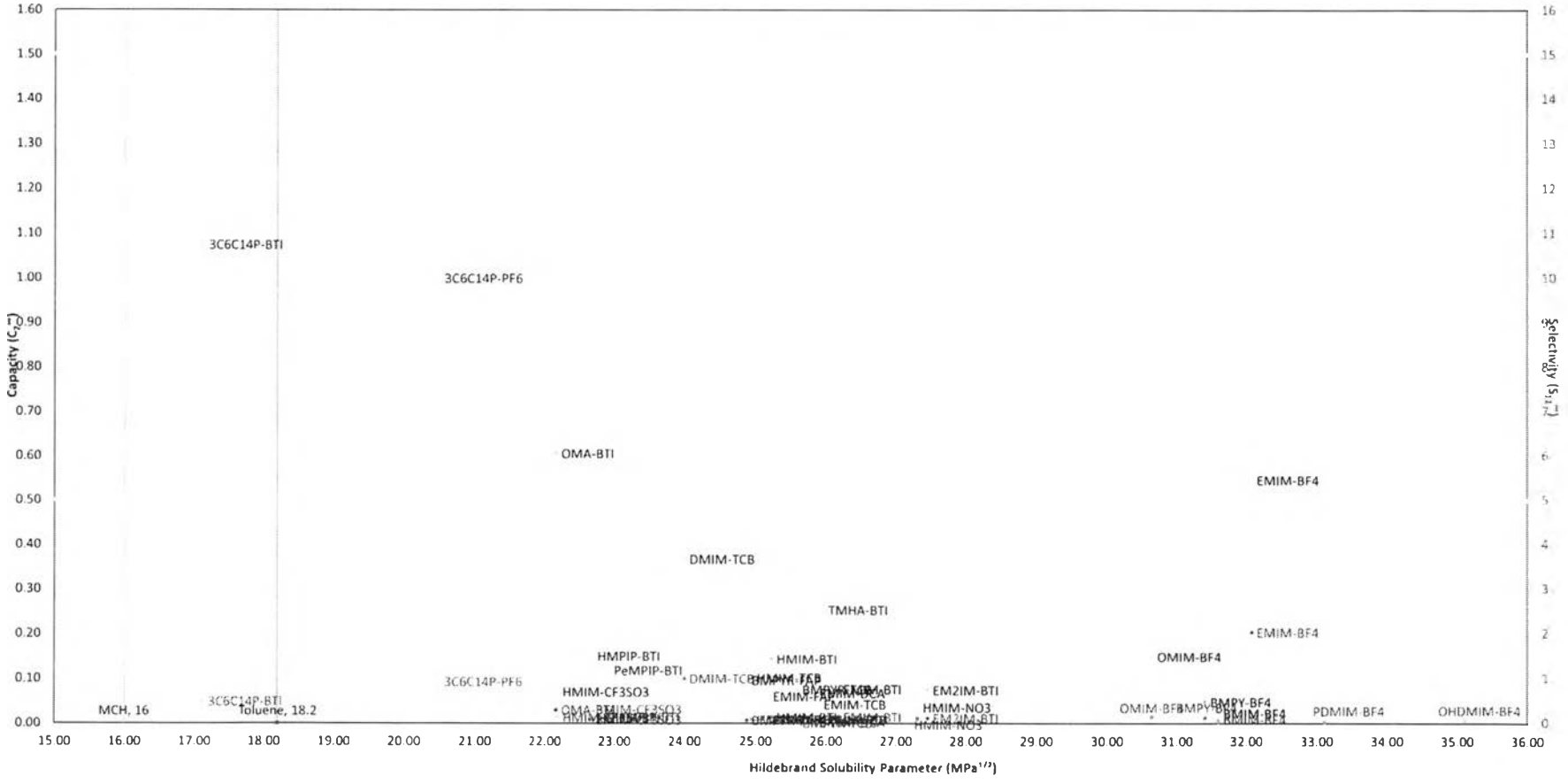

Figure B21 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the toluene + MCH mixture. MCH is the target solute

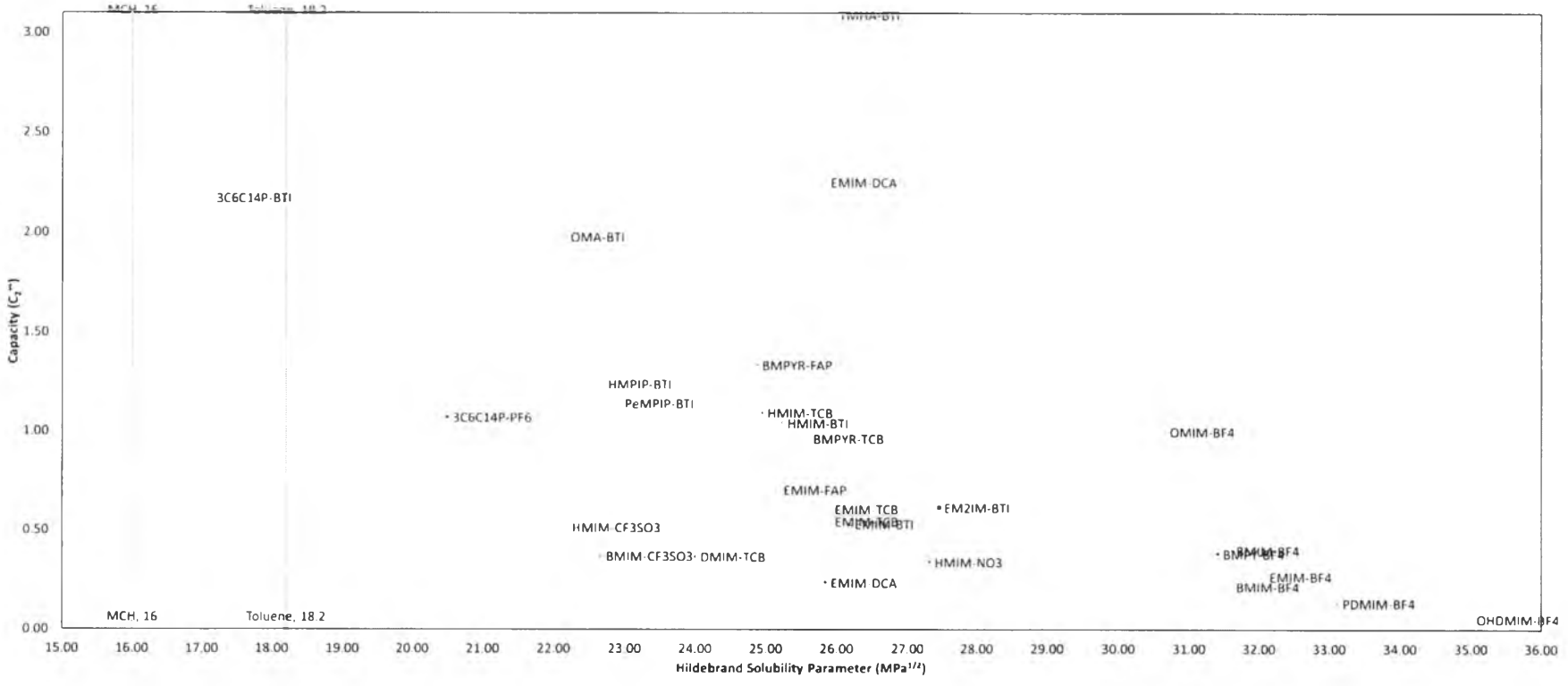

Figure B22 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^{∞}) of ILs (toluene as target solute) (Toluene + MCH mixture).

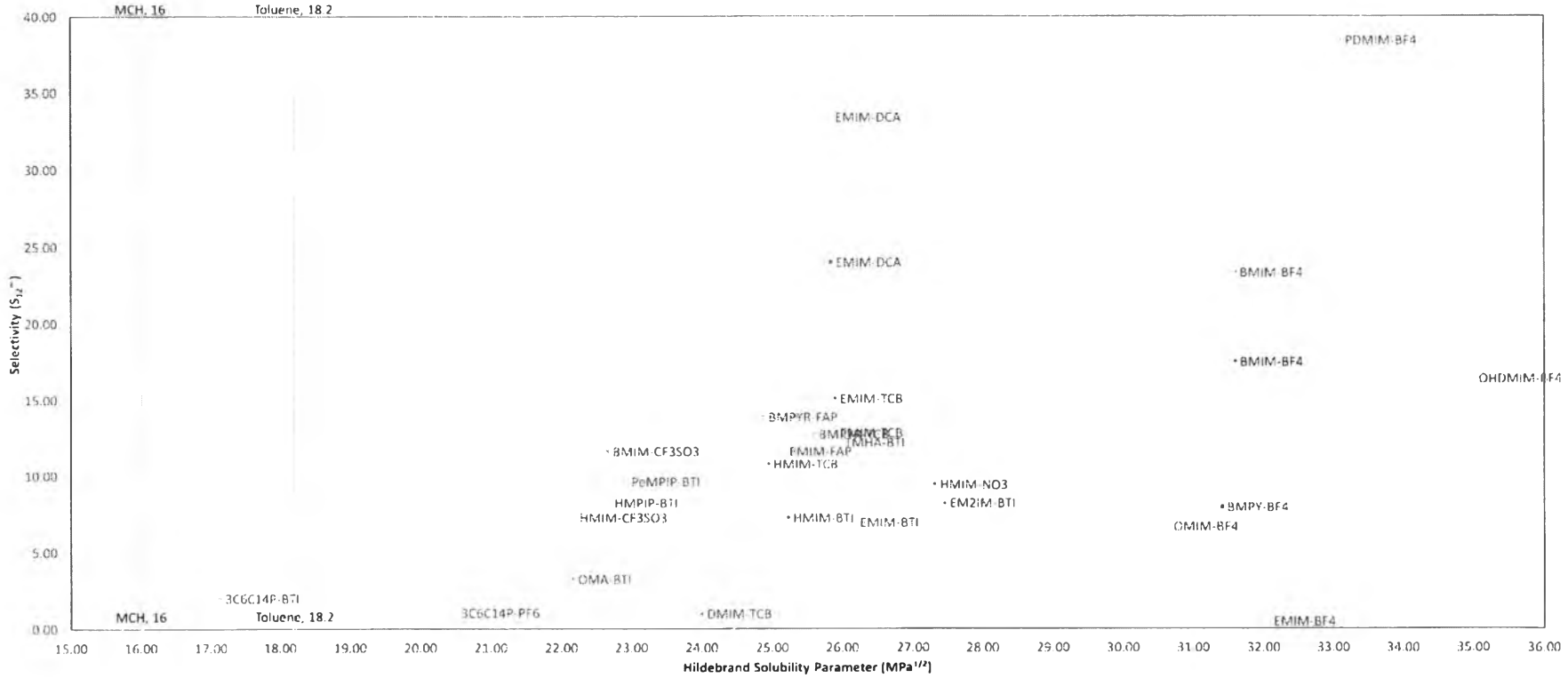

Figure B23 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (toluene as target solute) (Toluene + MCH mixture).

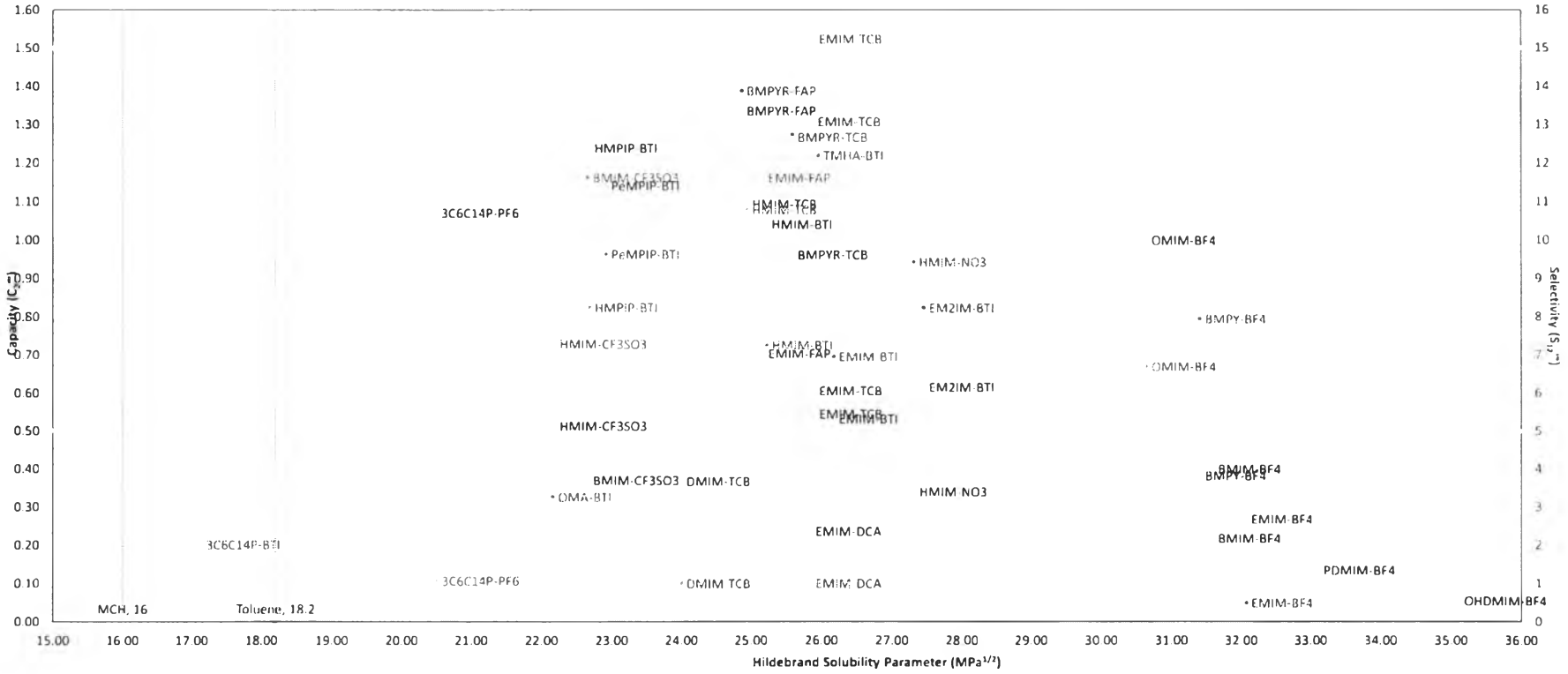

Figure B24 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the toluene + MCH mixture. Toluene is the target solute.

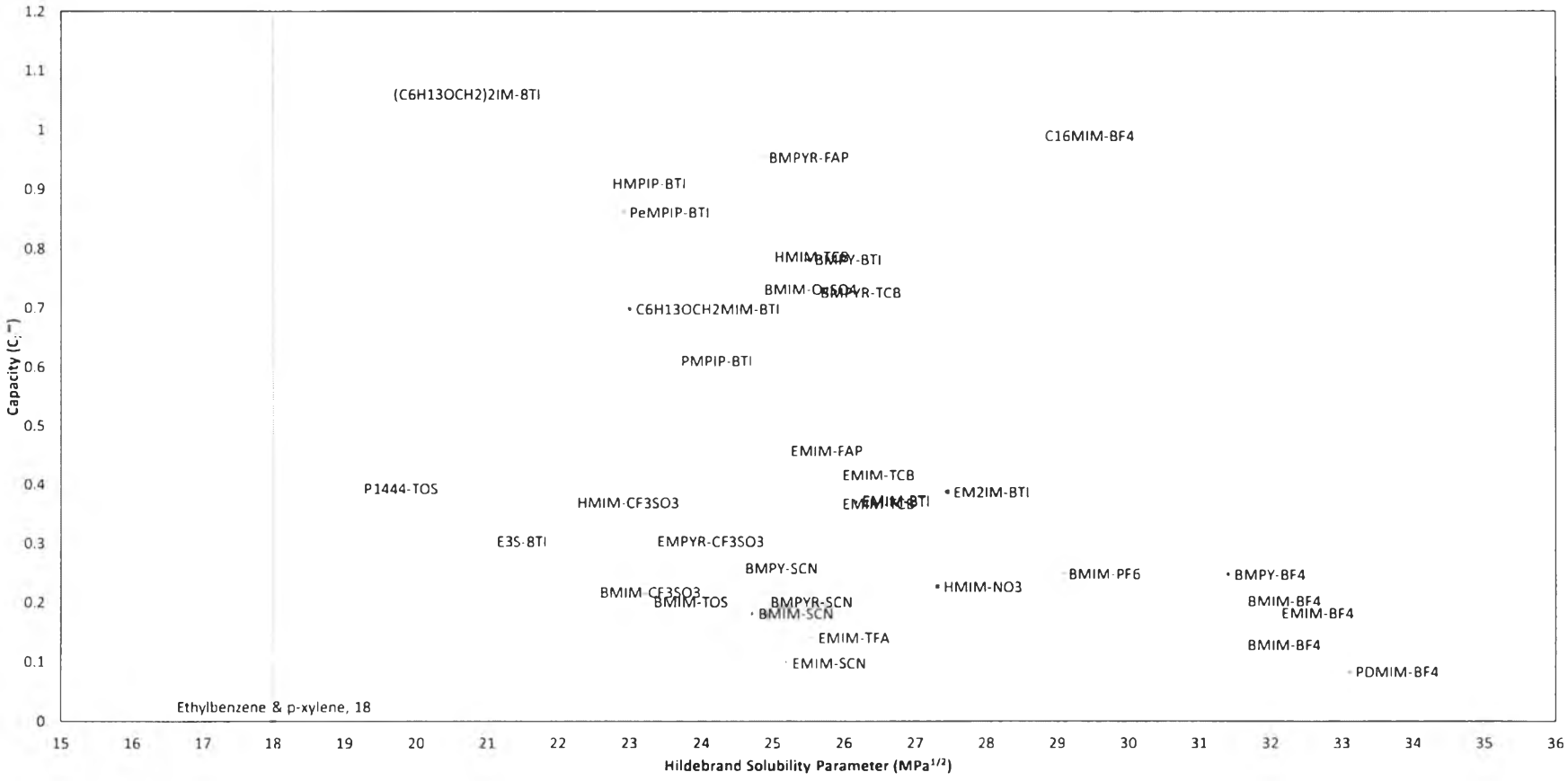

Figure B25 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^{∞}) of ILs (PX as target solute) (EB + PX mixture).

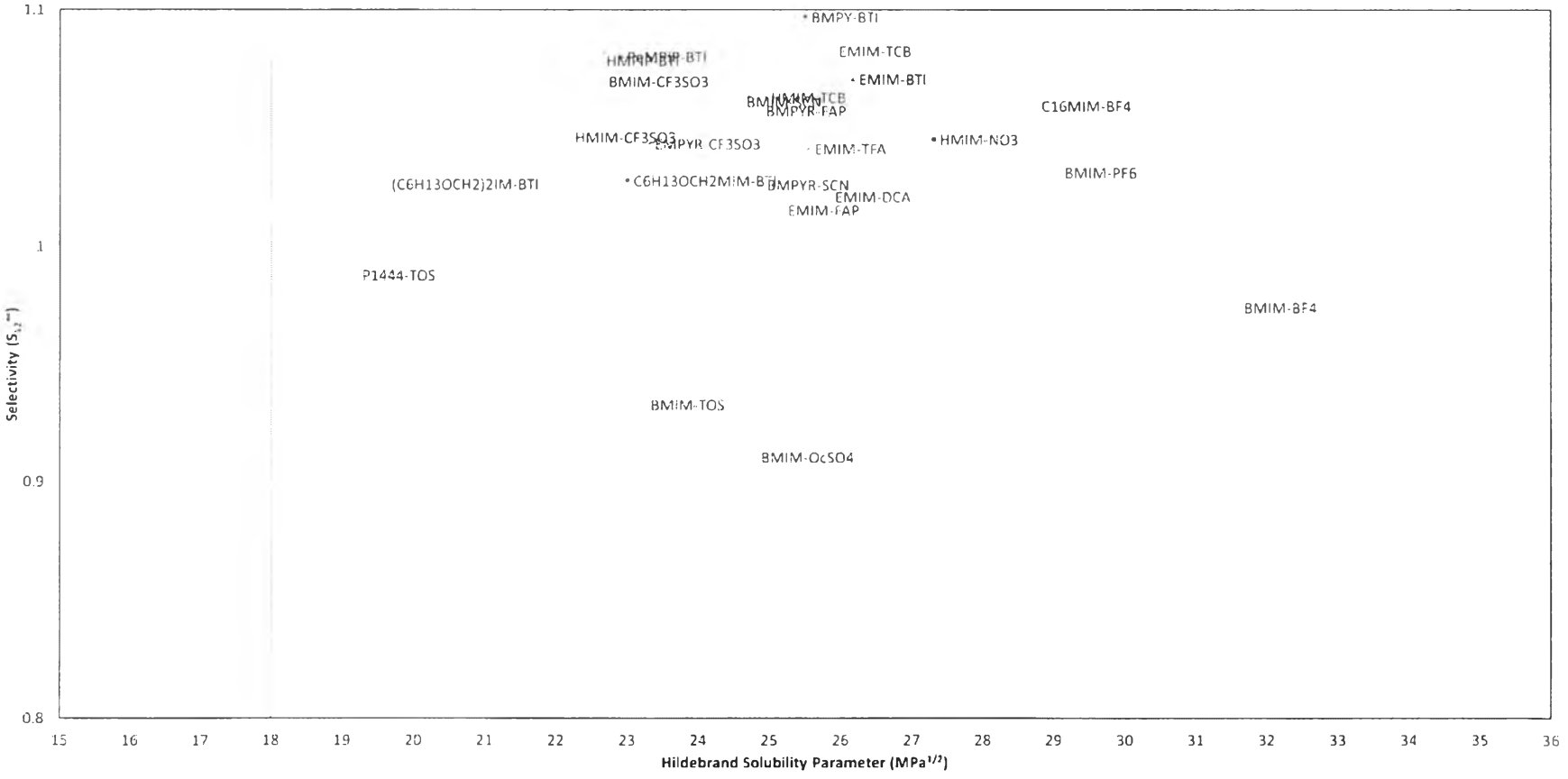

Figure B26 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (PX as target solute) (EB + PX mixture).

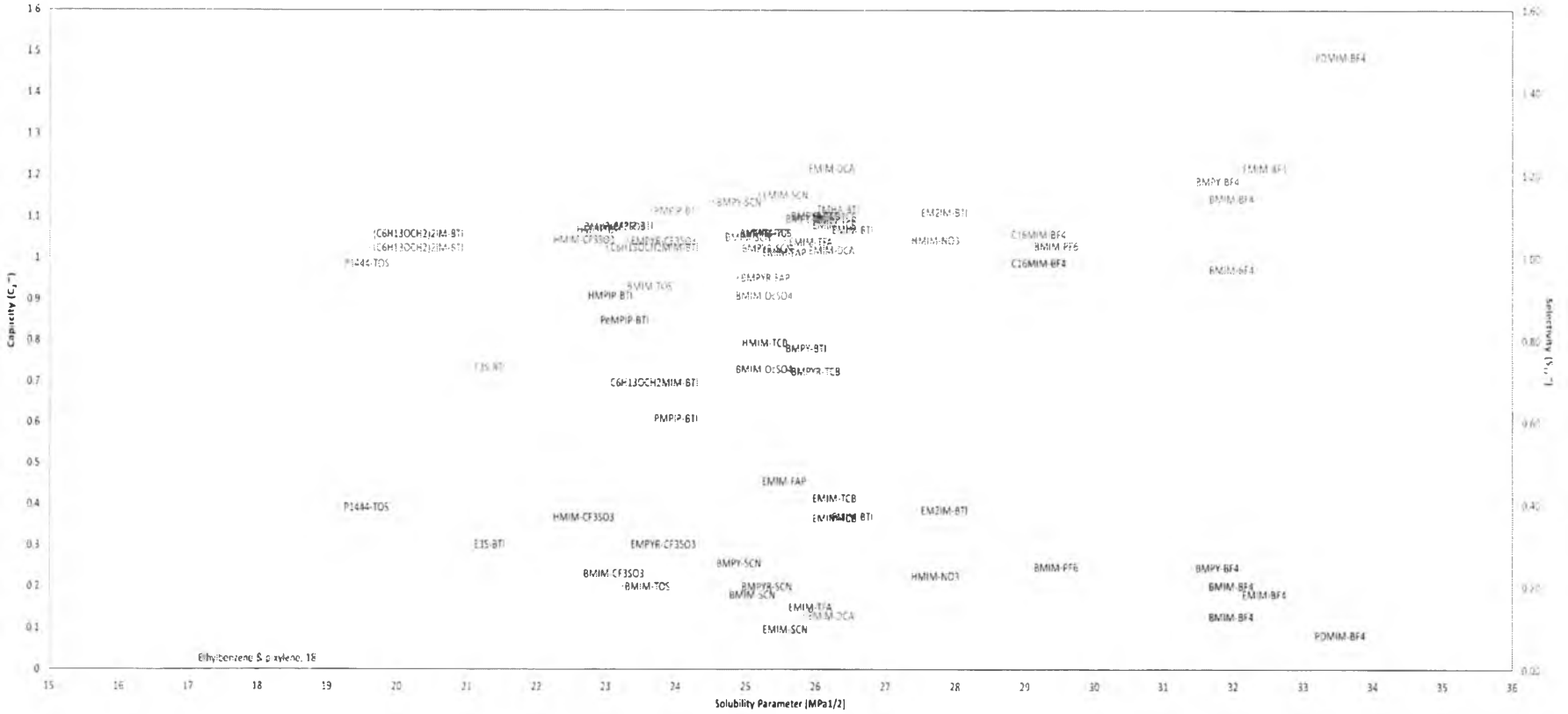

Figure B27 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the EB + PX mixture. PX is the target solute..

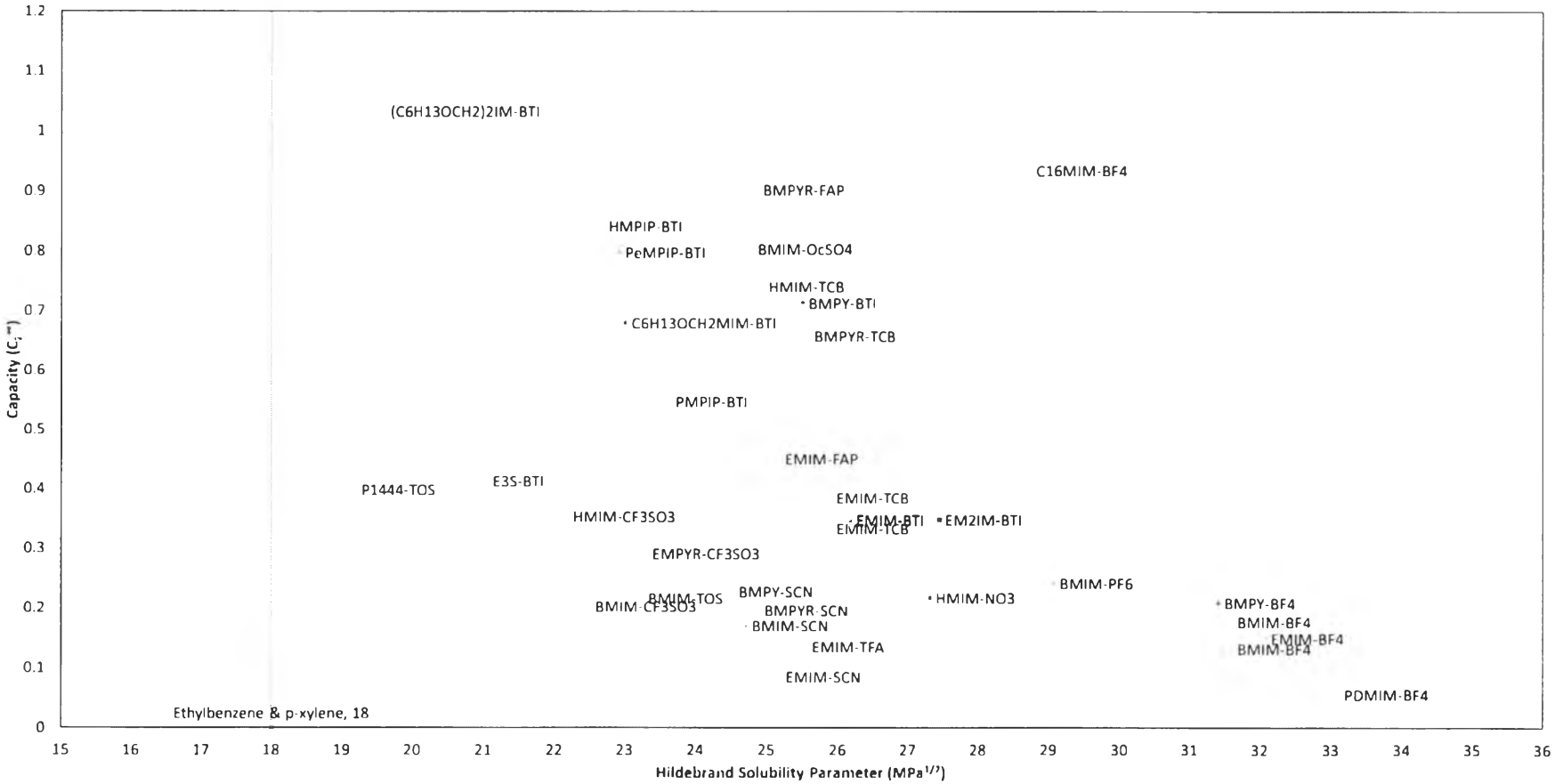

Figure B28 Hildebrand solubility parameters of ILs in *x-axis* vs Capacity (C_2^∞) of ILs (EB as target solute) (EB + PX mixture).

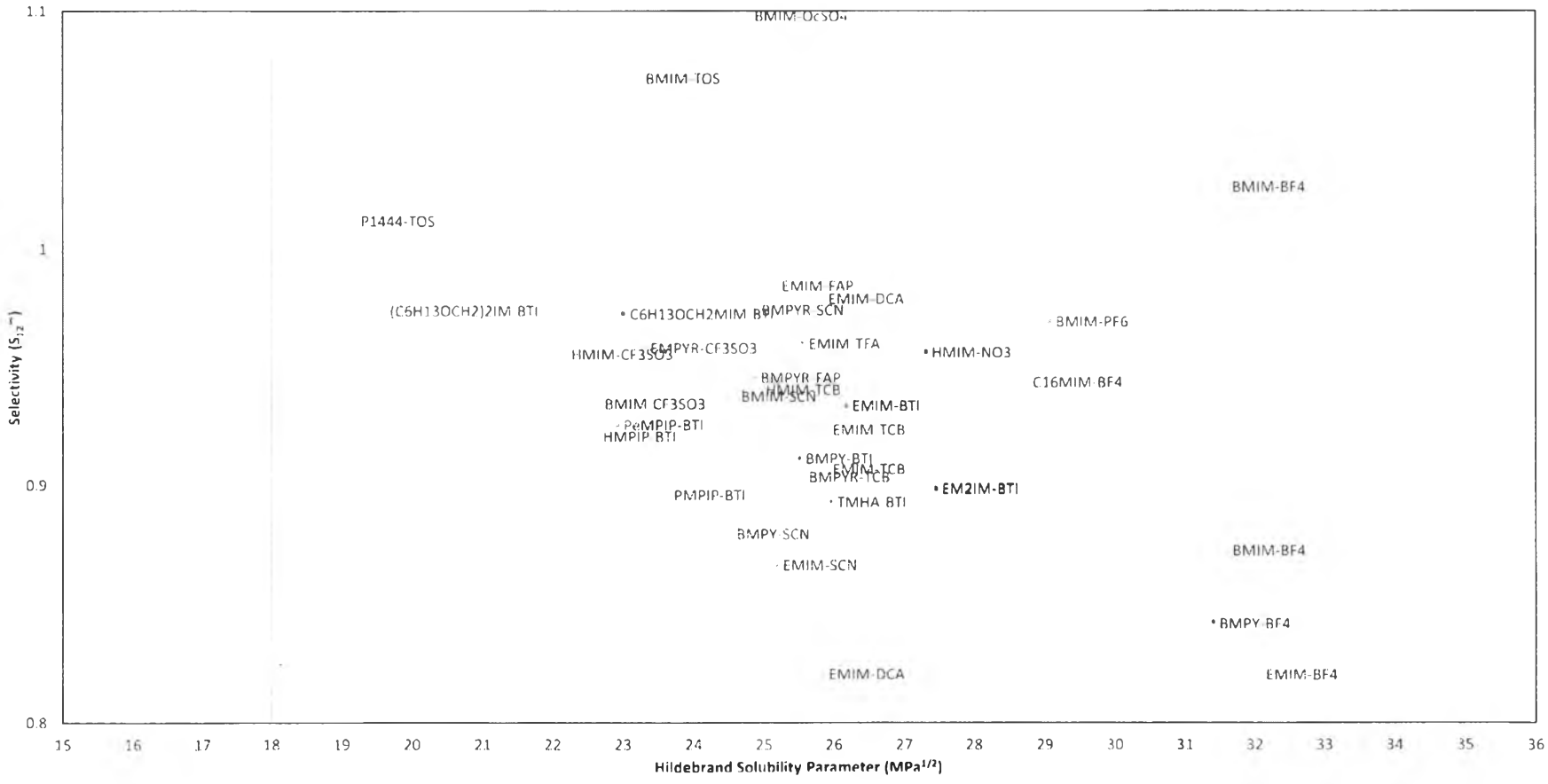

Figure B29 Hildebrand solubility parameters of ILs in *x-axis* vs Selectivity (S_{12}^{∞}) of ILs in *y-axis* (EB as target solute) (EB + PX mixture).

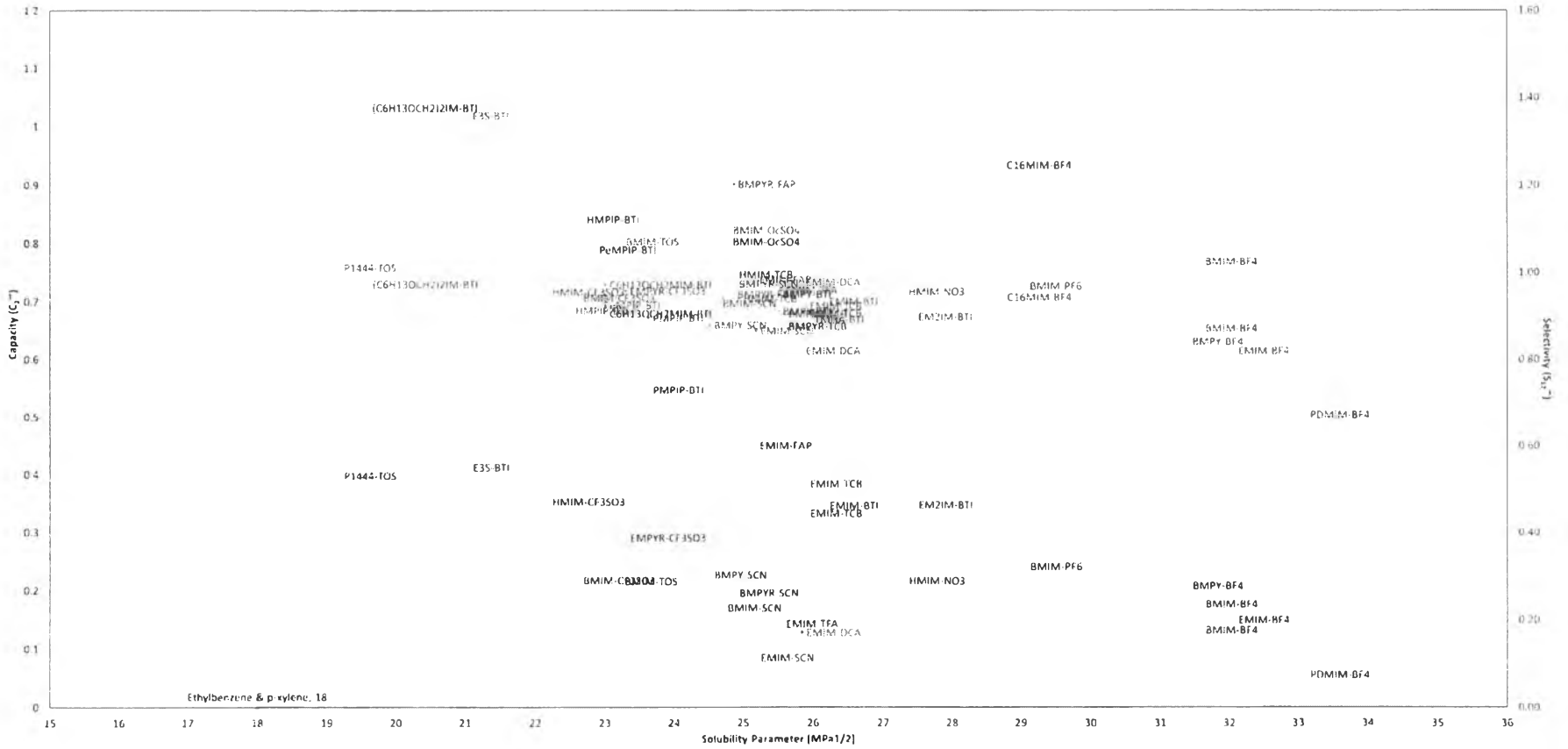

Figure B30 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the EB + PX mixture. EB is the target solute.

Table B2 Feasible IL candidates in water + ethanol mixture

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 2-12 capacity	min-max 1-6 selectivity	References
27	P1444-TOS	19.18	1.62	0.43	Doman'ska (2010)-4
16	(C6H13OCH2)2IM-BTI	19.60	0.23	0.98	Doman'ska (2009)-2
18	E3S-BTI	21.05	0.23	0.49	Doman'ska (2009)-3
14	BMIM-CF3SO3	22.66	1.11	1.19	Doman'ska (2008)-2
23 $MPa^{1/2}$, Minimum Hildebrand Solubility Parameter					
15	C6H13OCH2MIM-BTI	23.01	0.23	0.36	Doman'ska (2009)
30	BMIM-TOS	23.25	5.85	2.11	Doman'ska (2010)-6
17	EMPYR-CF3SO3	23.31	0.59	0.62	Doman'ska (2009)-2
26	PMPIP-BTI	23.64	0.20	0.45	Doman'ska (2010)-3
24	DMIM-TCB	24.00	0.37	1.00	Doman´ska (2010)
25	HMIM-SCN	24.24	1.75	1.48	Doman'ska (2010)-2
83	EMIM-EtSO4	24.45	4.35	3.87	Sumartschenkowa (2006)
28	BMPY-SCN	24.53	3.54	2.47	Doman'ska (2010)-5

Table B2 Feasible IL candidates in water + ethanol mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 2-12 capacity	min-max 1-6 selectivity	References
20	BMIM-SCN	24.72	3.74	2.78	Doman'ska (2009)-5
51	OMIM-BTI	24.76	0.24	0.42	Kato (2005)
33	BMPYR-FAP	24.88	0.08	0.28	Doman´ska (2012)
29	BMPYR-SCN	24.89	3.54	2.13	Doman'ska (2010)-5
13	EMIM-SCN	25.19	3.74	3.74	Doman'ska (2008)
19	BMPY-BTI	25.52	0.21	0.07	Doman'ska (2009)-4
12	EMIM-TFA	25.56	9.68	3.41	Doman'ska (2007)
31	BMPYR-TCB	25.60	0.39	0.58	Doman´ska (2011)
76	EMIM-DCA	25.84	2.50	2.00	Mutelet (2010)-1, Ge (2008)
32	EMIM-TCB	25.90	0.45	0.71	Doman'ska (2011)-2
54	EMIM-BTI	26.18	0.29	0.59	Krummen (2002)
90	MMIM-DMP	27.08	11.11	1.70	Zhao (2006)
47	BMIM-BF4	31.60	0.38	0.42	Juan Zhang (2007)
47 $MPa^{1/2}$, Hildebrand Solubility Parameter of Water					

Table B3 Feasible IL candidates in ethanol + hexane mixture

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
50 $MPa^{1/2}$, Maximum Hildebrand Solubility Parameter					
3	3C6C14P-Cl	15.56	1.32	1.02	Banerjee (2006)
64	3C6C14P-FAP	16.22	0.75	0.51	Letcher (2005)-4
5	3C6C14P-BTI	17.13	1.14	0.89	Banerjee (2006)
66	3C6C14P-BTI	17.13	0.72	0.77	Letcher (2008)
85	3C6C14P-BTI	17.13	0.61	0.66	Tumba (2013)
27	P1444-TOS	19.18	3.80	185.56	Doman'ska (2010)-4
16	(C6H13OCH2)2IM-BTI	19.60	0.23	0.74	Doman'ska (2009)-2
84	3C6C14P-PF6	20.50	0.33	0.78	Tumba (2012)
21 $MPa^{1/2}$, Maximum Hildebrand Solubility Parameter					
18	E3S-BTI	21.05	0.47	13.30	Doman'ska (2009)-3
39	OMA-BTI	22.16	1.03	1.17	Gwala (2010)
14	BMIM-CF3SO3	22.66	0.93	38.88	Doman'ska (2008)-2
78	HMPIP-BTI	22.69	0.47	3.90	Paduszyn´ski (2013)

Table B3 Feasible IL candidates in ethanol + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
77	PeMPIP-BTI	22.93	0.48	5.19	Paduszyn´ski (2013)
15	C6H13OCH2MIM-BTI	23.01	0.63	5.26	Doman'ska (2009)
4	3C6C14P-BF4	23.02	0.17	0.17	Banerjee (2006)
67	BMPY-TOS	23.06	1.03	49.15	Letcher (2009)
30	BMIM-TOS	23.25	2.77	138.94	Doman'ska (2010)-6
17	EMPYR-CF3SO3	23.31	0.95	53.14	Doman'ska (2009)-2
26	PMPIP-BTI	23.64	0.46	11.57	Doman'ska (2010)-3
24	DMIM-TCB	24.00	0.37	1.00	Doman´ska (2010)
28	BMPY-SCN	24.53	1.43	153.30	Doman'ska (2010)-5
20	BMIM-SCN	24.72	1.35	304.17	Doman'ska (2009)-5
51	OMIM-BTI	24.76	0.57	3.31	Kato (2005)
72	BMIM-OcSO4	24.80	1.84	28.97	Mutelet (2006)
33	BMPYR-FAP	24.88	0.28	3.24	Doman´ska (2012)
34	HMIM-TCB	24.95	0.84	10.95	Doman´ska (2012)-2

Table B3 Feasible IL candidates in ethanol + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
88	EMIM-FAP	25.18	0.26	3.27	Zhi-Cheng Tan (2011)
13	EMIM-SCN	25.19	1.00	327.00	Doman'ska (2008)
50	HMIM-BTI	25.23	0.53	4.83	Kato (2005),Liebert (2008)
45	HMIM-BTI	25.23	0.48	3.90	Heintz (2006)
19	BMPY-BTI	25.52	2.78	42.86	Doman'ska (2009)-4
12	EMIM-TFA	25.56	2.84	239.00	Doman'ska (2007)
31	BMPYR-TCB	25.60	1.52	1.38	Doman´ska (2011)
43	BMIM-BTI	25.71	0.53	8.19	Heintz (2005)
74	EMIM-DCA	25.84	5.67	466.75	Mutelet (2010)
76	EMIM-DCA	25.84	1.25	199.12	Mutelet (2010)-1, Ge (2008)
52	BMPYR-BTI	25.88	0.48	7.64	Kato (2005)
32	EMIM-TCB	25.90	0.63	21.39	Doman'ska (2011)-2
89	EMIM-TCB	25.90	0.54	13.68	Zhi-Cheng Tan (2011)
75	TMHA-BTI	25.96	0.44	6.12	Mutelet (2010)

Table B3 Feasible IL candidates in ethanol + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
75	TMHA-BTI	25.96	0.44	6.12	Mutelet (2010)
26 $MPa^{1/2}$, Hildebrand Solubility Parameter of Ethanol					
41	EMIM-BTI	26.18	0.59	16.04	Heintz (2002)
11	EMIM-BTI	26.18	0.59	15.96	Didenhofen (2003)
54	EMIM-BTI	26.18	0.50	14.51	Krummen (2002)
46	BM3A-BTI	26.44	0.44	8.67	Heintz (2006)-2
49	HMIM-NO3	27.32	1.69	101.95	Kan (2012)
42	EM2IM-BTI	27.46	0.43	11.87	Heintz (2002)
10	EM2IM-BTI	27.46	0.43	31.36	Didenhofen (2003)
60	HMIM-PF6	28.60	0.58	12.95	Letcher (2003)-2
73	C16MIM-BF4	28.75	0.56	1.22	Mutclet (2007)
48	OMIM-BF4	30.65	2.00	17.20	Juan Zhang (2007)
38	OMIM-BF4	30.65	0.71	9.48	Foco (2006)
44	OMIM-BF4	30.65	0.57	7.09	Heintz (2005)-2

Table B3 Feasible IL candidates in ethanol + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
31 $MPa^{1/2}$, Maximum Hildebrand Solubility Parameter					
37	HMIM-BF4	31.12	0.60	21.08	Foco (2006)
40	BMPY-BF4	31.41	0.51	32.34	Heintz (2001)
9	BMPY-BF4	31.41	0.50	36.70	Didenhofen (2003)
47	BMIM-BF4	31.60	0.91	59.91	Juan Zhang (2007)
36	BMIM-BF4	31.60	0.44	42.17	Foco (2006)
80	BMIM-BF4	31.60	0.44	58.83	Revelli (2009)

Table B4 Feasible IL candidates in benzene + hexane mixture

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.3-2.1 capacity	min-max 6-42 selectivity	References
3	3C6C14P-Cl	15.56	2.43	1.88	Banerjee (2006)
64	3C6C14P-FAP	16.22	4.76	3.24	Letcher (2005)-4
66	3C6C14P-BTI	17.13	2.70	2.88	Letcher (2008)
85	3C6C14P-BTI	17.13	2.56	2.79	Tumba (2013)
5	3C6C14P-BTI	17.13	2.45	1.91	Banerjee (2006)
18 $MPa^{1/2}$, Minimum Hildebrand Solubility Parameter					
18.8 $MPa^{1/2}$, Hildebrand Solubility Parameter of Benzene					
27	P1444-TOS	19.18	0.65	31.90	Doman'ska (2010)-4
16	(C6H13OCH2)2IM-BTI	19.60	1.64	5.30	Doman'ska (2009)-2
84	3C6C14P-PF6	20.50	1.22	2.84	Tumba (2012)
18	E3S-BTI	21.05	0.93	26.48	Doman'ska (2009)-3
39	OMA-BTI	22.16	3.23	3.67	Gwala (2010)
86	HMIM-CF3SO3	22.19	0.71	15.19	Yang (2008)

Table B4 Feasible IL candidates in benzene + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.3-2.1 capacity	min-max 6-42 selectivity	References
14	BMIM-CF3SO3	22.66	0.65	26.84	Doman'ska (2008)-2
69	BMIM-CF3SO3	22.66	0.56	21.78	Ming-Lan Ge (2007)
78	HMPIP-BTI	22.69	1.55	12.84	Paduszyn´ski (2013)
77	PeMPIP-BTI	22.93	1.47	16.09	Paduszyn´ski (2013)
15	C6H13OCH2MIM-BTI	23.01	1.25	10.42	Doman'ska (2009)
4	3C6C14P-BF4	23.02	2.69	2.70	Banerjee (2006)
67	BMPY-TOS	23.06	1.03	49.15	Letcher (2009)
6	OMIM-Cl	23.19	0.50	8.64	David (2003)
30	BMIM-TOS	23.25	0.50	24.86	Doman'ska (2010)-6
17	EMPYR-CF3SO3	23.31	0.71	39.57	Doman'ska (2009)-2
26	PMPIP-BTI	23.64	1.10	27.78	Doman'ska (2010)-3
65	3BMP-MeSO4	23.72	1.00	11.23	Letcher (2007)
8	OMIM-MDEGSO4	23.85	0.68	8.84	Deenadayalu (2006)
24	DMIM-TCB	24.00	0.37	1.00	Doman´ska (2010)

Table B4 Feasible IL candidates in benzene + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.3-2.1 capacity	min-max 6-42 selectivity	References
56	EMIM-EtSO4	24.45	0.37	41.20	Krummen (2002)
28	BMPY-SCN	24.53	0.60	64.46	Doman'ska (2010)-5
20	BMIM-SCN	24.72	0.47	106.10	Doman'ska (2009)-5
51	OMIM-BTI	24.76	1.64	9.57	Kato (2005)
72	BMIM-OcSO4	24.80	1.69	26.64	Mutelet (2006)
62	BMIM-OcSO4	24.80	0.70	5.08	Letcher (2005)-2
63	BMIM-MDEGSO4	24.80	0.49	39.66	Letcher (2005)-3
33	BMPYR-FAP	24.88	1.76	20.13	Doman´ska (2012)
34	HMIM-TCB	24.95	1.38	18.00	Doman´ska (2012)-2
88	EMIM-FAP	25.18	1.01	12.97	Zhi-Cheng Tan (2011)
13	EMIM-SCN	25.19	0.29	95.34	Doman'ska (2008)
61	HMIM-BTI	25.23	1.48	12.36	Letcher (2005)
50	HMIM-BTI	25.23	1.41	12.88	Kato (2005),Liebert (2008)
45	HMIM-BTI	25.23	1.28	10.51	Heintz (2006)

Table B4 Feasible IL candidates in benzene + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.3-2.1 capacity	min-max 6-42 selectivity	References
19	BMPY-BTI	25.52	1.46	22.55	Doman'ska (2009)-4
12	EMIM-TFA	25.56	0.36	30.65	Doman'ska (2007)
31	BMPYR-TCB	25.60	1.52	1.38	2.54665
31	BMPYR-TCB	25.60	1.28	23.65	Doman´ska (2011)
55	BMIM-BTI	25.71	1.14	16.73	Krummen (2002)
43	BMIM-BTI	25.71	1.14	17.50	Heintz (2005)
74	EMIM-DCA	25.84	1.15	94.85	Mutelet (2010)
76	EMIM-DCA	25.84	0.39	61.72	Mutelet (2010)-1, Ge (2008)
52	BMPYR-BTI	25.88	1.27	20.31	Kato (2005)
32	EMIM-TCB	25.90	0.88	29.91	Doman'ska (2011)-2
89	EMIM-TCB	25.90	0.76	19.20	Zhi-Cheng Tan (2011)
75	TMHA-BTI	25.96	1.25	17.34	Mutelet (2010)
7	EMIM-BTI	26.18	1.29	26.87	Deenadayalu (2005)
11	EMIM-BTI	26.18	0.85	23.17	Didenhofen (2003)

Table B4 Feasible IL candidates in benzene + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.3-2.1 capacity	min-max 6-42 selectivity	References
41	EMIM-BTI	26.18	0.85	23.16	Heintz (2002)
54	EMIM-BTI	26.18	0.84	24.49	Krummen (2002)
53	MMIM-BTI	26.42	0.75	31.02	Krummen (2002)
46	BM3A-BTI	26.44	0.73	14.49	Heintz (2006)-2
49	HMIM-NO3	27.32	0.53	31.66	Kan (2012)
59	EMMIM-BTI	27.46	0.92	25.41	Letcher (2003)
42	EM2IM-BTI	27.46	0.92	25.05	Heintz (2002)
10	EM2IM-BTI	27.46	0.90	66.10	Didenhofen (2003)
60	HMIM-PF6	28.60	0.97	21.84	Letcher (2003)-2
28, Minimum Hildebrand Solubility Parameter					
73	C16MIM-BF4	28.75	1.27	2.75	Mutelet (2007)
48	OMIM-BF4	30.65	1.43	12.29	Juan Zhang (2007)
44	OMIM-BF4	30.65	0.84	10.42	Heintz (2005)-2

Table B4 Feasible IL candidates in benzene + hexane mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.3-2.1 capacity	min-max 6-42 selectivity	References
38	OMIM-BF4	30.65	0.78	10.49	Foco (2006)
57	HMIM-BF4	31.12	1.04	23.02	Letcher (2003)
37	HMIM-BF4	31.12	0.61	21.49	Foco (2006)
9	BMPY-BF4	31.41	0.62	45.12	Didenhofen (2003)
58	BMPY-BF4	31.41	0.61	39.79	Letcher (2003)
40	BMPY-BF4	31.41	0.61	39.08	Heintz (2001)
47	BMIM-BF4	31.60	0.67	43.93	Juan Zhang (2007)
79	BMIM-BF4	31.60	0.58	37.27	Qing Zhou (2006)
80	BMIM-BF4	31.60	0.45	60.86	Revelli (2009)
36	BMIM-BF4	31.60	0.42	40.30	Foco (2006)
70	EMIM-BF4	32.07	0.46	49.49	Ming-Lan Ge (2008)
35	EMIM-BF4	32.07	0.42	57.73	Foco (2006)
68	PDMIM-BF4	33.11	0.22	90.77	Ming-Hui Wang (2007)

Table B5 Feasible IL candidates in toluene + MCH mixture

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
85	3C6C14P-BTI	17.13	2.17	2.0217	Tumba (2013)
18 $MPa^{1/2}$, Minimum Hildebrand Solubility Parameter					
18.2 $MPa^{1/2}$, Hildebrand Solubility Parameter of Toluene					
84	3C6C14P-PF6	20.50	1.07	1.0714	Tumba (2012)
39	OMA-BTI	22.16	1.98	3.2670	Gwala (2010)
86	HMIM-CF3SO3	22.19	0.51	7.2919	Yang (2008)
69	BMIM-CF3SO3	22.66	0.37	11.6296	Ming-Lan Ge (2007)
78	HMPIP-BTI	22.69	1.24	8.2503	Paduszyn´ski (2013)
77	PeMPIP-BTI	22.93	1.14	9.6445	Paduszyn´ski (2013)
24	DMIM-TCB	24.00	0.37	1.0000	Doman´ska (2010)
33	BMPYR-FAP	24.88	1.34	13.8829	Doman´ska (2012)
34	HMIM-TCB	24.95	1.09	10.7959	Doman´ska (2012)-2
88	EMIM-FAP	25.18	0.70	11.6252	Zhi-Cheng Tan (2011)

Table B5 Feasible IL candidates in toluene + MCH mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
50	HMIM-BTI	25.23	1.04	7.2615	Kato (2005),Liebert (2008)
31	BMPYR-TCB	25.60	1.52	1.3767	Doman´ska (2011)
74	EMIM-DCA	25.84	2.25	33.4162	Mutelet (2010)
32	EMIM-TCB	25.90	2.60	2.4017	Doman'ska (2011)-2
89	EMIM-TCB	25.90	0.55	12.8342	Zhi-Cheng Tan (2011)
75	TMHA-BTI	25.96	3.09	12.2031	Mutelet (2010)
75	TMHA-BTI	25.96	3.09	12.2031	Mutelet (2010)
11	EMIM-BTI	26.18	0.53	6.9604	Didenhofen (2003)
49	HMIM-NO3	27.32	0.34	9.4354	Kan (2012)
10	EM2IM-BTI	27.46	0.62	8.2346	Didenhofen (2003)
28 $MPa^{1/2}$, Minimum Hildebrand Solubility Parameter					
48	OMIM-BF4	30.65	1.00	6.7000	Juan Zhang (2007)
9	BMPY-BF4	31.41	0.38	7.9522	Didenhofen (2003)
47	BMIM-BF4	31.60	0.40	17.4800	Juan Zhang (2007)

Table B5 Feasible IL candidates in toluene + MCH mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 5-15 selectivity	References
79	BMIM-BF4	31.60	0.35	17.5087	Qing Zhou (2006)
80	BMIM-BF4	31.60	0.22	23.3341	Revelli (2009)
70	EMIM-BF4	32.07	0.27	0.4906	Ming-Lan Ge (2008)
68	PDMIM-BF4	33.11	0.13	38.4160	Ming-Hui Wang (2007)
87	OHDMIM-BF4	35.11	0.05	16.3948	Zhang (2009)

Table B6 Feasible IL candidates in EB + PX mixture

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 0.5-1.5 selectivity	References
18 $MPa^{1/2}$, Minimum Hildebrand solubility Parameter and Hildebrand Solubility Parameter of EB & PX					
16	(C6H13OCH2)2IM-BTI	19.60	1.03	0.974173	Doman'ska (2009)-2
18	E3S-BTI	21.05	0.41	1.359504	Doman'ska (2009)-3
86	HMIM-CF3SO3	22.19	0.35	0.955799	Yang (2008)
69	BMIM-CF3SO3	22.66	0.22	0.934782	Ming-Lan Ge (2007)
15	C6H13OCH2MIM-BTI	23.01	0.68	0.972807	Doman'ska (2009)
17	EMPYR-CF3SO3	23.31	0.29	0.958345	Doman'ska (2009)-2
20	BMIM-SCN	24.72	0.17	0.940273	Doman'ska (2009)-5
72	BMIM-OcSO4	24.80	0.80	1.098070	Mutelet (2006)
33	BMPYR-FAP	24.88	0.90	0.945821	Doman´ska (2012)
34	HMIM-TCB	24.95	0.74	0.940740	Doman´ska (2012)-2
88	EMIM-FAP	25.18	0.45	0.98467	Zhi-Cheng Tan (2011)

Table B6 Feasible IL candidates in EB + PX mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 0.5-1.5 selectivity	References
13	EMIM-SCN	25.19	0.09	0.86638	Doman'ska (2008)
19	BMPY-BTI	25.52	0.71	0.91155	Doman'ska (2009)-4
12	EMIM-TFA	25.56	0.14	0.96026	Doman'ska (2007)
30	BMIM-TOS	23.25	0.22	1.07166	Doman'ska (2010)-6
74	EMIM-DCA	25.84	3.55	0.820540	Mutelet (2010)
89	EMIM-TCB	25.90	0.33	0.907	Zhi-Cheng Tan (2011)
75	TMHA-BTI	25.96	6.33	0.89297	Mutelet (2010)
41	EMIM-BTI	26.18	0.35	0.933797	Heintz (2002)
11	EMIM-BTI	26.18	0.35	0.93409	Didenhofen (2003)
49	HMIM-NO3	27.32	0.22	0.95661	Kan (2012)
42	EM2IM-BTI	27.46	0.35	0.898954	Hcintz (2002)
10	EM2IM-BTI	27.46	0.35	0.89839	Didenhofen (2003)
73	C16MIM-BF4	28.75	0.93	0.94392	Mutelet (2007)
71	BMIM-PF6	29.07	0.24	0.96959	Mutelet (2005)

Table B6 Feasible IL candidates in EB + PX mixture (Continued)

No.	Ionic Liquids (ILs)	Hildebrand Solubility Parameter ($MPa^{1/2}$)	min-max 0.5-1.5 capacity	min-max 0.5-1.5 selectivity	References
30 $MPa^{1/2}$, Maximum Hildebrand Solubility Parameter					
40	BMPY-BF4	31.41	0.21	0.84166	Heintz (2001)
9	BMPY-BF4	31.41	0.21	0.84222	Didenhofen (2003)
79	BMIM-BF4	31.60	0.18	0.87256	Qing Zhou (2006)
80	BMIM-BF4	31.60	0.13	1.02622	Revelli (2009)
70	EMIM-BF4	32.07	0.15	0.82035	Ming-Lan Ge (2008)
68	PDMIM-BF4	33.11	0.06	0.67228	Ming-Hui Wang (2007)

Appendix C Derivation of Hildebrand Solubility Parameter Model for ILs

According to the previous work, Kulajanpeng (2014) proposed the Hildebrand solubility parameter model for ILs (δ_{IL}) as shown in Equation 2.5 which was used to predict the Hildebrand solubility parameters at 298.15 K.

Where, subscript i, j, and k represent alkyl chain groups, cation groups, and anion groups respectively. n_i describes the number of groups of type i, C_i is the contribution of group i to the overall solubility parameter value, and b is a constant value.

Group contributions (GC) of the Hildebrand solubility parameter model for ILs is extended from 39 different ILs, which consists of 5 alkyl chains, 8 cations and 20 anions groups (34 independent variables including a constant term). The verification of group contributions (GC) of the Hildebrand solubility parameter model for ILs provides a good fit with a value of 0.319%AARD (percent average absolute relative deviation) and 3.29 (the maximum relative deviation) between the experimental and predicted solubility parameter values as shown in Figure 2.11.

For example, 1-Ethyl-3-methylimidazolium tetrafluoroborate, [EMIM][BF_4] is composed of of 2 CH_3 groups (i), 1 CH_2 group (i), 1 Imidazolium [IM] cation group (j) , and 1 Tetrafluoroborate [BF_4] anion group (k). By using Equation 2.5 and Table 2.7, the Hildebrand solubility parameter of [EMIM][BF_4] is 32.07 $MPa^{1/2}$.

Appendix D Supplementary Data in Verification of Mixture Step

- Original NRTL binary parameters (Table D1)

Table D1 Original NRTL binary parameters of four case studies

Mixture		α_{ij}	**Original NRTL binary parameters**	
Component *i*	**Component *j***		A_{ij} (K^{-1})	A_{ji} (K^{-1})
Ethanol	Water	0.3008	-61.44	675.02
Hexane	Ethanol	0.05	1057.25	-669.95
Hexane	Benzene	0.11	-692.33	1194.61
MCH	Toluene	0.3	-43.24	134.06
EB	PX	No data		

Appendix E Calculation of Original NRTL Binary Parameters

NRTL binary parameters are generally catagorized into two factors: (1) Nonrandomness Factors (α_l) and (2) Energy Parameters (e.g. g_{ij} or a_{ij} and b_{ij}). However, a diversity of NRTL binary parameters must be concerned and altered the same type as the original NRTL binary parameters (A_{ij}) for inputting in ICAS program so that Equation E1 and E2 are proposed to calculate.

$$A_{ij}\,(K^{-1}) = (g_{ij})\,/R\;\;;R = 8.314\;J/mol\cdot K \tag{E1}$$

$$A_{ij}\,(K^{-1}) = [a_{ij}(T) + b_{ij}]/R\;\;;R = 8.314\;J/mol\cdot K\;and\;T = 298\;K \tag{E2}$$

Appendix F Supplementary Data in Verification of IL Step

- Original NRTL binary parameters (Table F1-F4)
- Critical properties of ILs (Table F5-F11)

Table F1 Original NRTL binary parameters of water + ethanol mixture

Mixture		α_{ij}	Original NRTL binary parameters	
Component *i*	**Component *j***		A_{ij} (K^{-1})	A_{ji} (K^{-1})
Ethanol	Water	0.3008	-61.439	675.02
Ethanol	[MMIM][DMP]	0.2508	-2427.36	-713.89
Water	[MMIM][DMP]	0.1038	-3156.39	-870.00
Ethanol	[EMIM][DCA]	0.75	846.05	-247.08
Water	[EMIM][DCA]	0.827	1149.51	-314.29
Ethanol	[EMIM][EtSO4]	0.3018	-558.98	87932.04
Water	[EMIM][EtSO4]	0.996	-210.39	-486.61

Table F2 Original NRTL binary parameters of ethanol + hexane mixture

Mixture		α_{ij}	Original NRTL binary parameters	
Component *i*	**Component *j***		A_{ij} (K^{-1})	A_{ji} (K^{-1})
Hexane	Ethanol	0.05	1057.25	-669.95
Hexane	[EMIM][BTI]	0.05	4123.17	-1218.43
Ethanol	[EMIM][BTI]	0.05	5093.82	-3151.31
Hexane	[BMIM][BTI]	0.19	1937.70	162.38
Ethanol	[BMIM][BTI]	0.19	2481.36	-1378.40

Table F3 Original NRTL binary parameters of benzene + hexane mixture

Mixture		α_{ij}	Original NRTL binary parameters	
Component *i*	**Component *j***		A_{ij} (K^{-1})	A_{ji} (K^{-1})
Hexane	Benzene	0.11	-692.33	1194.61
Hexane	[EMIM][EtSO4]	0.11	7505.29	864.69
Benzene	[EMIM][EtSO4]	0.11	2309.60	-762.69
Hexane	[BMIM][BTI]	0.3	1739.72	588.89
Benzene	[BMIM][BTI]	0.3	3883.57	-51.48

Table F4 Original NRTL binary parameters of toluene + MCH mixture

Mixture		α_{ij}	Original NRTL binary parameters	
Component *i*	**Component *j***		A_{ij} (K^{-1})	A_{ji} (K^{-1})
MCH	Toluene	0.3	-43.24	134.06
MCH	[HMIM][TCB]	0.2	2121.99	204.24
Toluene	[HMIM][TCB]	0.2	2078.30	-716.97
MCH	[HMIM][BTI]	0.2	2558.60	471.80
Toluene	[HMIM][BTI]	0.2	1348.10	-89.60

Table F5 Critical properties of [MMIM][DMP]

[MMIM][DMP]		
IUPAC name	1,3-dimethylimidazolium dimethylphosphate	
global formula		
CAS No.	654058-04-5	
MW (g/mol)	222.2	
Density (ρ_L, g/cm^3)	1.2633	
Critical Properties	Tb (K)	590
	Tc (K)	816.8
	Pc (bar)	27.2
	Vc (cm^3/mol)	626.8
	ω	0.5973
	Zc	0.2509

Table F6 Critical properties of [EMIM][BTI]

[EMIM][BTI]		
IUPAC name	1-ethyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	
global formula	C8H11N3F6S2O4	
CAS No.	174899-82-2	
MW (g/mol)	391.30	
Density (ρ_L, g/cm^3)	1.5221	
Critical Properties	Tb (K)	816.70
	Tc (K)	1249.30
	Pc (bar)	32.65
	Vc (cm^3/mol)	875.90
	ω	0.2157
	Zc	0.2753

Table F7 Critical properties of [EMIM][EtSO4]

[EMIM][EtSO4]		
IUPAC name	1-ethyl-3-methylimidazolium ethylsulfate	
global formula	C8H16N2SO4	
CAS No.	342573-75-5	
MW (g/mol)	236.300	
Density (ρ_L, g/cm^3)	1.2658	
Critical Properties	Tb (K)	712.70
	Tc (K)	1067.50
	Pc (bar)	40.46
	Vc (cm^3/mol)	659.80
	ω	0.374
	Zc	0.301

Table F8 Critical properties of [EMIM][DCA]

[EMIM][DCA]		
IUPAC name	1-ethyl-3-methylimidazolium dicyanamide	
global formula	C8H11N5	
CAS No.	370865-89-7	
MW (g/mol)	177.2	
Density (ρ_L, g/cm^3)	1.0879	
Critical Properties	Tb (K)	737.2
	Tc (K)	999
	Pc (bar)	29.1
	Vc (cm^3/mol)	597.8
	ω	0.7661
	Zc	0.2095

Table F9 Critical properties of [BMIM][BTI]

[BMIM][BTI]		
IUPAC name	1-butyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	
global formula	C10H15N3F6S2O4	
CAS No.	174899-83-3	
MW (g/mol)	419.40	
Density (ρ_L, g/cm^3)	1.4483	
Critical Properties	Tb (K)	862.40
	Tc (K)	1269.90
	Pc (bar)	27.65
	Vc (cm^3/mol)	990.10
	ω	0.3004
	Zc	0.2592

Table F10 Critical properties of [HMIM][BTI]

[HMIM][BTI]		
IUPAC name	1-hexyl-3-methylimidazolium bis[(trifluoromethyl)sulfonyl]imide	
global formula	C12H19N3F6S2O4	
CAS No.	382150-50-7	
MW (g/mol)	447.40	
Density (ρ_L, g/cm^3)	1.3893	
Critical Properties	Tb (K)	908.20
	Tc (K)	1292.80
	Pc (bar)	23.89
	Vc (cm^3/mol)	1104.40
	ω	0.3893
	Zc	0.2454

Table F11 Critical properties of [HMIM][TCB]

[HMIM][TCB]		
IUPAC name	1-Hexyl-3-methylimidazolium tetracyanoborate	
global formula	C14H19BN6	
cas number	1240857-50-4	
MW (g/mol)	282.159	
Density (ρ_L, g/cm^3)	1.0274	
Critical Properties	Tb (K)	1043.7
	Tc (K)	1276.8
	Pc (bar)	17.0
	Vc (cm^3/mol)	1000.6
	ω	1.3661
	Zc	0.158

Appendix G Supplementary Data in Simulation Comparison

- **Water + Ethanol Mixture**
  - EG (Figure G1, Table G1 - G4)
  - [MMIM][DMP] (Figure G2, Table G5 - G9)
  - [EMIM][DCA] (Figure G3, Table G10 - G14)
  - [EMIM][EtSO4] (Figure G4, Table G15 - G19)
- **Ethanol + Hexane Mixture**
  - Sulfolane (Figure G5, Table G20 - G23)
  - [EMIM][BTI] (Figure G6, Table G24 - G28)
  - [BMIM][BTI] (Figure G7, Table G29 - G33)
- **Benzene + Hexane Mixture**
  - NMP (Figure G8, Table G34 - G37)
  - [EMIM][EtSO4] (Figure G9, Table G38 - G42)
  - [BMIM][BTI] (Figure G10, Table G43 - G47)
- **Toluene + MCH Mixture**
  - NMP (Figure G11, Table G48 - G51)
  - [HMIM][TCB] (Figure G12, Table G52 - G56)
  - [HMIM][BTI] (Figure G13, Table G57 - G61)

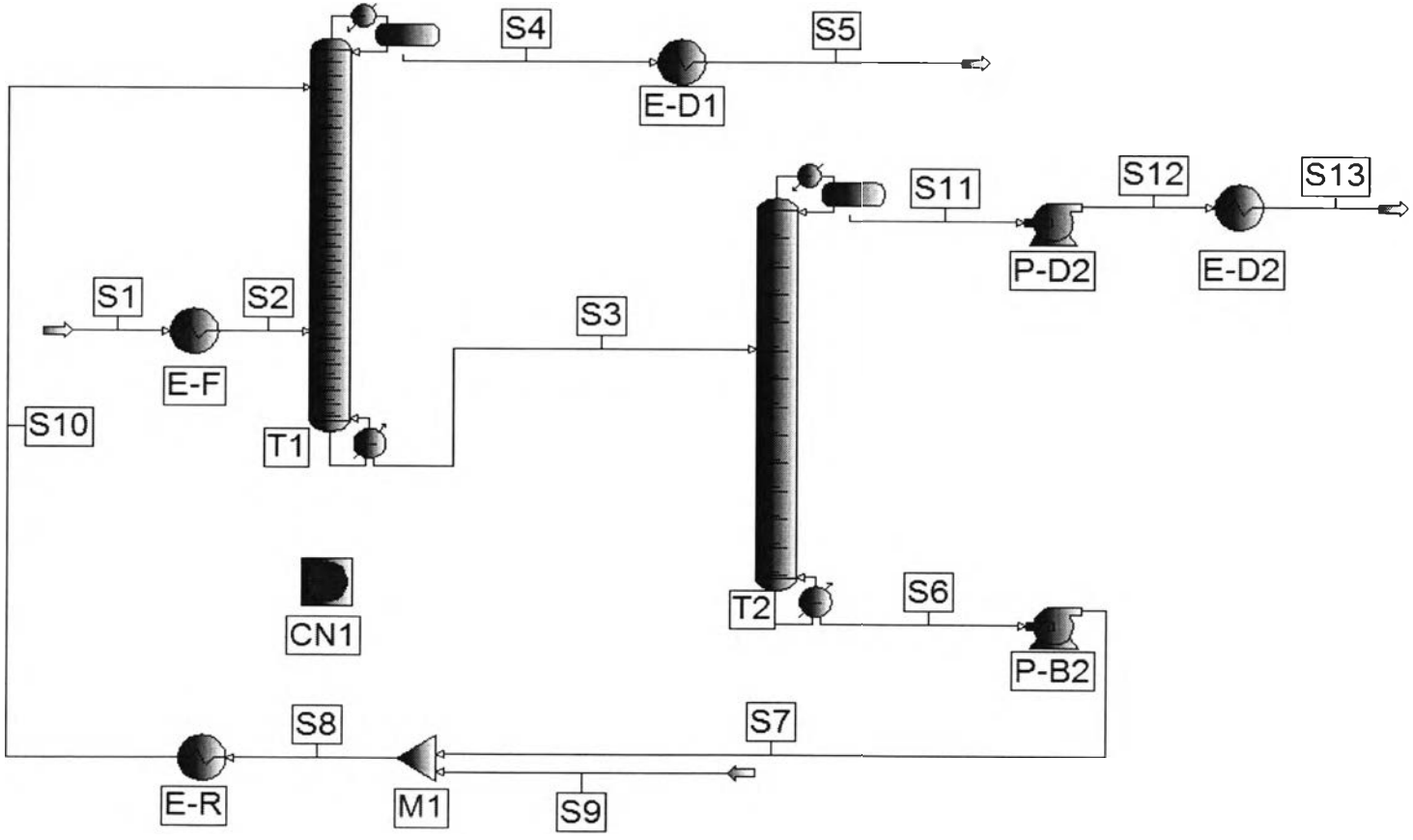

Figure G1 CS process flowsheet using EG in water + ethanol mixture.

Table G1 Distillation column properties of the CS process using EG in water + ethanol mixture

Column Name	**Unit**	**T1**	**T2**
Column Description			
Condenser Duty	MM WATT	-2.9889	-0.9227
Reboiler Duty	MM WATT	3.9097	0.7843
Column Total Molar Feed	KG-MOL/HR	410.0861	249.9614
Column Total Wt. Feed	KG/HR	21131.2750	13762.4051
Column Condenser Pres	KPA	100.0000	20.0000
Column Condenser Temp	C	77.9707	58.9314
Column Reflux Rate	KG-MOL/HR	0.0000	35.1778
Column Reflux Ratio		0.7318	0.8819

Table G2 Pump properties of the CS process using EG in water + ethanol mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	80.0000	80.0000
Head	M	8.0581	8.3455
Work	KW	0.2860	0.0164

Table G3 Heat exchanger properties of the CS process using EG in water + ethanol mixture

Hx Name	**Unit**	**E-D1**	**E-D2**	**E-F**	**E-R**
Hx Description					
Duty	MM WATT	0.3432	0.0301	0.4355	0.8220
MTD	C	14.8293	8.7175	65.4246	76.3167

Table G4 Stream table of the CS process using EG in water + ethanol mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S2	S3
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	25	78	58.93141645	58.93529036	30	78	155.0733358
Pressure	KPA	100	100	20	100	100	100	100
Total Mass Rate	KG/HR	8091.663905	13039.61113	723.5339536	723.5339536	723.5339536	8091.663905	13762.40513
Flowrate	KG-MOL/HR	200.0001624	210.0859431	39.88735097	39.88735097	39.88735097	200.0001624	249.9613723
Total Weight Comp. Rates	KG/HR							
ETHANOL		7371.052129	1.149640221e-008	7.372434259	7.372434259	7.372434259	7371.052129	7.372434136
WATER		720.611776	0.03578510929	715.5095728	715.5095728	715.5095728	720.611776	715.54535
EG		0						
Total Weight Comp. Fractions								
ETHANOL		0.9109439314	8.816522284e-013	0.01018947932	0.01018947932	0.01018947932	0.9109439314	0.0005356937298
WATER		0.08905606863	2.744338688e-006	0.988909462	0.988909462	0.988909462	0.08905606863	0.0519927544
EG		0	0.9999972557	0.0009010586922	0.0009010586922	0.0009010586922	0	0.9474715519
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		160.0001299	2.495472579e-010	0.1600301312	0.1600301312	0.1600301312	160.0001299	0.1600301285
WATER		40.00003248	0.00198637544	39.71681716	39.71681716	39.71681716	40.00003248	39.7188031
EG		0	210.0839567	0.01050367891	0.01050367891	0.01050367891	0	210.082539
Composition								
ETHANOL		0.8	1.187834151e-012	0.004012052125	0.004012052125	0.004012052125	0.8	0.0006402194351
WATER		0.2	9.455061158e-006	0.9957246143	0.9957246143	0.9957246143	0.2	0.1588997642
EG		0	0.9999905449	0.0002633335795	0.0002633335795	0.0002633335795	0	0.8404600164

Table G4 Stream table of the CS process using EG in water + ethanol mixture (Continued)

Stream Name	Unit	S4	S5	S6	S7	S8	S9
Stream Description							
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	77.97066512	30	150.6819571	150.6938335	150.636793	25
Pressure	KPA	100	100	20	100	100	100
Total Mass Rate	KG/HR	7368.869899	7368.869899	13038.87116	13038.87116	13039.61113	6.206840134
Flowrate	KG-MOL/HR	160.1247332	160.1247332	210.0740213	210.0740213	210.0859431	0.1
Total Weight Comp. Rates	KG/HR						
ETHANOL		7363.679695	7363.679695	1.149875087e-008	1.149875087e-008	1.149640221e-008	0
WATER		5.102211118	5.102211118	0.03578525266	0.03578525266	0.03578510929	0
EG		0.08799290548					
Total Weight Comp. Fractions							
ETHANOL		0.9992956581	0.9992956581	8.818823908e-013	8.818823908e-013	8.816522284e-013	0
WATER		0.0006924007599	0.0006924007599	2.744505427e-006	2.744505427e-006	2.744338688e-006	0
EG		1.194116692e-005	1.194116692e-005	0.9999972555	0.9999972555	0.9999972557	1
Total Molar Comp. Rates	KG-MOL/HR						
ETHANOL		159.8400998	159.8400998	2.495982393e-010	2.495982393e-010	2.495472579e-010	0
WATER		0.2832157581	0.2832157581	0.001986383399	0.001986383399	0.00198637544	0
EG		0.001417676363	0.001417676363	210.0720349	210.0720349	210.0839567	0.1
Composition							
ETHANOL		0.9982224268	0.9982224268	1.188144245e-012	1.188144245e-012	1.187834151e-012	0
WATER		0.001768719625	0.001768719625	9.455635621e-006	9.455635621e-006	9.455061158e-006	0
EG		8.853575175e-006	8.853575175e-006	0.9999905444	0.9999905444	0.9999905449	1

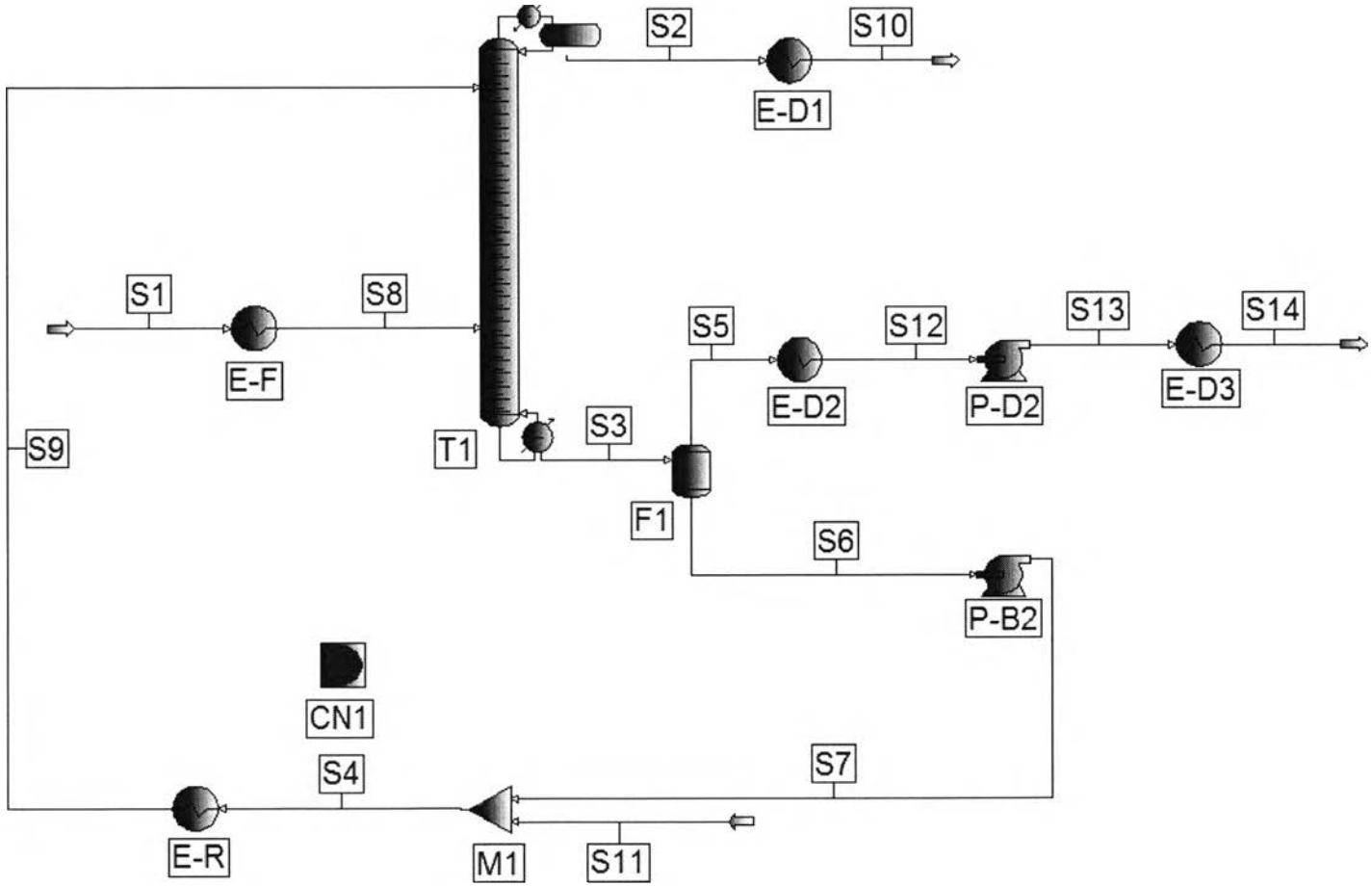

Figure G2 IL process flowsheet using [MMIM][DMP] in water + ethanol mixture.

Table G5 Distillation column properties of the IL process using [MMIM][DMP] in water + ethanol mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.1623
Reboiler Duty	MM WATT	3.2476
Column Total Molar Feed	KG-MOL/HR	240.0410
Column Total Wt. Feed	KG/HR	16980.6048
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	77.9710
Column Reflux Rate	KG-MOL/HR	133.2830
Column Reflux Ratio		0.8324

Table G6 Flash properties of the IL process using [MMIM][DMP] in water + ethanol mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	254.9971
Pressure	KPA	1.0000
DP	KPA	99.0000
Duty	MM WATT	0.6154

Table G7 Pump properties of the IL process using [MMIM][DMP] in water + ethanol mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	99.0000	99.0000
Head	M	8.1406	10.1211
Work	KW	0.1970	0.0199

Table G8 Heat exchanger properties of the ILn process using [MMIM][DMP] in water + ethanol mixture

Hx Name	**Unit**	**E-D1**	**E-D2**	**E-D3**	**E-F**	**E-R**
Hx Description						
Duty	MM WATT	0.3432	0.6200	0.0248	0.4355	0.1758
MTD	C	14.8294	273.3712	102.0833	65.4246	114.0617

Table G9 Stream table of the IL process using [MMIM][DMP] in water + ethanol mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	25	30	25	5.803236847	5.806522355	30	77.97096781
Pressure	KPA	100	100	100	1	100	100	100
Total Mass Rate	KG/HR	8091.663905	7368.723406	0.2221999969	722.9404819	722.9404819	722.9404819	7368.723406
Flowrate	KG-MOL/HR	200.0001624	160.1199969	0.001	39.88016449	39.88016449	39.88016449	160.1199969
Total Weight Comp. Rates	KG/HR							
ETHANOL		7371.052129	7363.681807	0	7.370322147	7.370322147	7.370322147	7363.681807
WATER		720.611776	5.041598771	0	715.5701588	715.5701588	715.5701588	5.041598771
[MMIM][DMP]		0	0	0.2221999969	8.852555819e-007	8.852555819e-007	8.852555819e-007	0
Total Weight Comp. Fractions								
ETHANOL		0.9109439314	0.9993158111	0	0.01019492245	0.01019492245	0.01019492245	0.9993158111
WATER		0.08905606863	0.0006841889012	0	0.9898050763	0.9898050763	0.9898050763	0.0006841889012
[MMIM][DMP]		0	0	1	1.224520696e-009	1.224520696e-009	1.224520696e-009	0
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		160.0001299	159.8401457	0	0.1599842845	0.1599842845	0.1599842845	159.8401457
WATER		40.00003248	0.2798512615	0	39.7201802	39.7201802	39.7201802	0.2798512615
[MMIM][DMP]		0	0	0.001	3.984048578e-009	3.984048578e-009	3.984048578e-009	0
Composition								
ETHANOL		0.8	0.9982522404	0	0.004011625493	0.004011625493	0.004011625493	0.9982522404
WATER		0.2	0.001747759598	0	0.9959883744	0.9959883744	0.9959883744	0.001747759598
[MMIM][DMP]		0	0	1	9.990050515e-011	9.990050515e-011	9.990050515e-011	0

Table G9 Stream table of the IL process using [MMIM][DMP] in water + ethanol mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid
Temperature	C	160.9884488	255.0916278	254.9971241	254.9971241	255.097375	78	78
Pressure	KPA	100	100	1	1	100	100	100
Total Mass Rate	KG/HR	9611.881374	8888.940876	722.9404819	8888.940888	8888.940888	8091.663905	8888.940876
Flowrate	KG-MOL/HR	79.92098504	40.04081955	39.88016449	40.04082056	40.04082056	200.0001624	40.04081955
Total Weight Comp. Rates	KG/HR							
ETHANOL		7.372839741	0.002518355362	7.370322147	0.002517598321	0.002517598321	7371.052129	0.002518355362
WATER		716.2865613	0.7163840819	715.5701588	0.7164029249	0.7164029249	720.611776	0.7163840819
[MMIM][DMP]		8888.221973	8888.221973	8.852555819e-007	8888.221967	8888.221967	0	8888.221973
Total Weight Comp. Fractions								
ETHANOL		0.0007670547995	2.833133212e-007	0.01019492245	2.832281542e-007	2.832281542e-007	0.9109439314	2.83313e-007
WATER		0.07452095312	8.059273787e-005	0.9898050763	8.059485759e-005	8.059485759e-005	0.08905606863	8.059273e-005
[MMIM][DMP]		0.9247119921	0.9999191239	1.224520696e-009	0.9999191219	0.9999191219	0	0.9999191239
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		0.1600389328	5.466481284e-005	0.1599842845	5.464838009e-005	5.464838009e-005	160.0001299	5.4664812e-005
WATER		39.75994658	0.0397653598	39.7201802	0.03976640574	0.03976640574	40.00003248	0.0397653598
[MMIM][DMP]		40.00099953	40.00099953	3.984048578e-009	40.0009995	40.0009995	0	40.00099953
Composition								
ETHANOL		0.002002464468	1.365227122e-006	0.004011625493	1.364816688e-006	1.364816688e-006	0.8	1.3652271e-006
WATER		0.4974906974	0.0009931205265	0.9959883744	0.0009931466237	0.0009931466237	0.2	0.0009931205265
[MMIM][DMP]		0.5005068382	0.9990055142	9.990050515e-011	0.9990054886	0.9990054886	0	0.9990055142

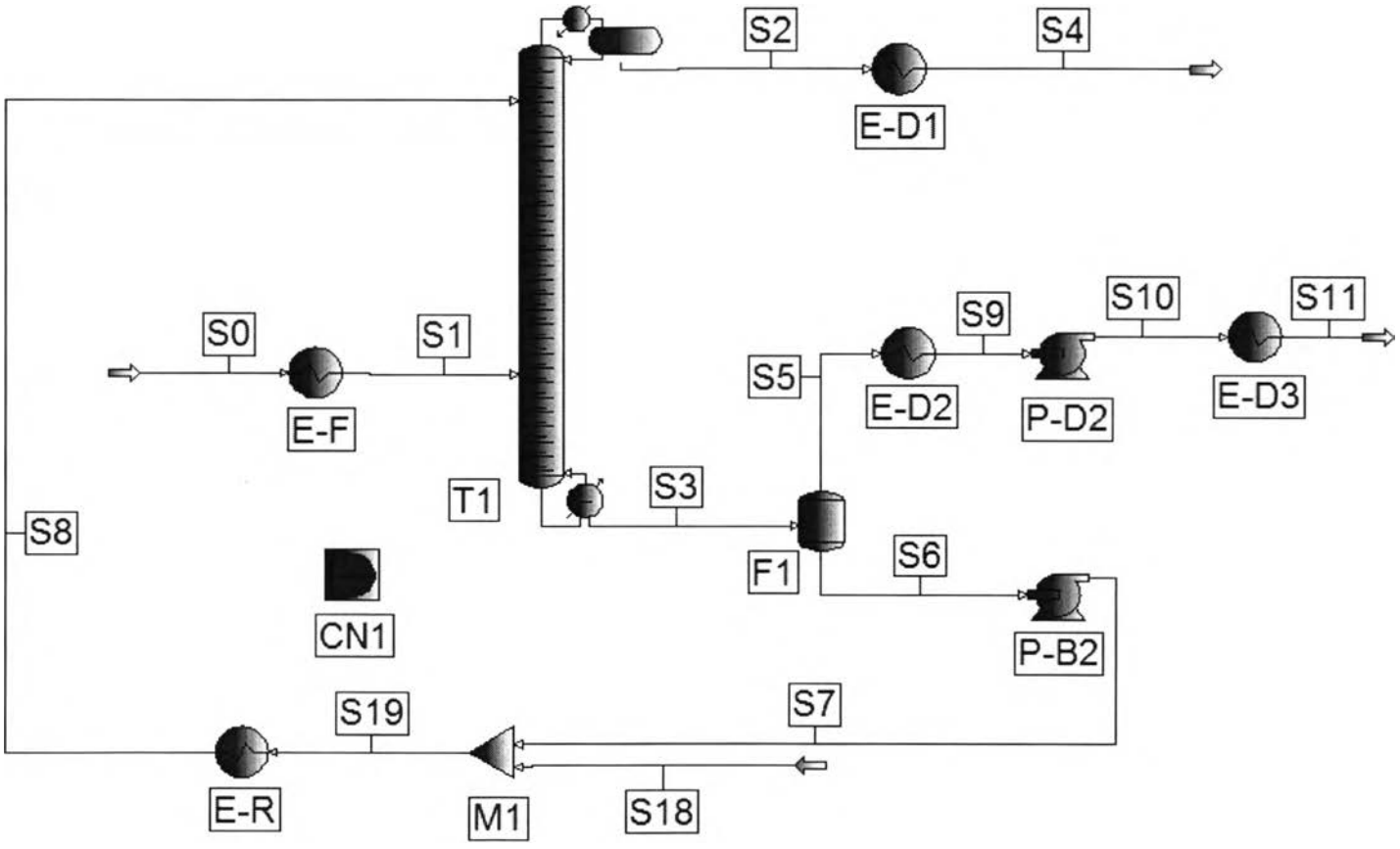

Figure G3 IL process flowsheet using [EMIM][DCA] in water + ethanol mixture.

Table G10 Distillation column properties of the IL process using [EMIM][DCA] in water + ethanol mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.2510
Reboiler Duty	MM WATT	3.3990
Column Total Molar Feed	KG-MOL/HR	290.0808
Column Total Wt. Feed	KG/HR	24041.2770
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	77.9767
Column Reflux Rate	KG-MOL/HR	141.4354
Column Reflux Ratio		0.8829

Table G11 Flash properties of the IL process using [EMIM][DCA] in water + ethanol mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	240.7885
Pressure	KPA	1.0000
DP	KPA	99.0000
Duty	MM WATT	0.7894

Table G12 Pump properties of the IL process using [EMIM][DCA] in water + ethanol mixture

Pump Name	**Unit**	**P1**	**P2**
Pump Description			
Pressure Gain	KPA	99.0000	99.0000
Head	M	9.6074	10.1216
Work	KW	0.4171	0.0199

Table G13 Heat exchanger properties of the separation process using [EMIM][DCA] in water + ethanol mixture

Hx Name	**Unit**	**E-F**	**E-D1**	**E-R**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	0.4355	0.3434	0.4187	0.6130	1.9284
MTD	C	65.4246	14.8310	109.2798	268.0933	1119.5007

Table G14 Stream table of the IL process using [EMIM][DCA] in water + ethanol mixture

Stream Name	Unit	S0	S1	S10	S11	S18	S19	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	25	78	5.965175025	30	25	240.8158912	77.97673616
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	8091.663905	8091.663905	721.4991491	721.4991491	0.1771999969	15949.61305	7370.164767
Flowrate	KG-MOL/HR	200.0001624	200.0001624	39.80027322	39.80027322	0.001	90.08060666	160.1998897
Total Weight Comp. Rates	KG/HR							
ETHANOL		7371.052129	7371.052129	7.366924313	7.366924313	0	0.003508327745	7363.685207
WATER		720.611776	720.611776	714.1322241	714.1322241	0	1.432780939	6.479559975
[EMIM][DCA]		0	0	7.046369e-007	7.046369277e-007	0.1771999969	15948.17676	0
Total Weight Comp. Fractions								
ETHANOL		0.9109439314	0.9109439314	0.010210579	0.01021057935	0	2.199631887e-007	0.9991208392
WATER		0.08905606863	0.08905606863	0.9897894197	0.9897894197	0	8.983170525e-005	0.000879160803
[EMIM][DCA]		0	0	9.766289e-010	9.766289102e-010	1	0.9999099483	0
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		160.0001299	160.0001299	0.1599105293	0.1599105293	0	7.615370034e-005	159.8402195
WATER		40.00003248	40.00003248	39.64036269	39.64036269	0	0.0795314287	0.3596702387
[EMIM][DCA]		0	0	3.976506e-009	3.976506432e-009	0.001	90.00099908	0
Composition								
ETHANOL		0.8	0.8	0.00401782	0.004017824913	0	8.453950652e-007	0.9977548659
WATER		0.2	0.2	0.995982175	0.995982175	0	0.0008828917971	0.002245134122
[EMIM][DCA]		0	0	9.99115e-011	9.991153603e-011	1	0.9991162628	0

Table G14 Stream table of the IL process using [EMIM][DCA] in water + ethanol mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid
Temperature	C	158.7093388	30	240.7884568	240.7884568	240.8188483	78	5.961885576
Pressure	KPA	100	100	1	1	100	100	1
Total Mass Rate	KG/HR	16671.11219	7370.164767	721.4991491	15949.613	15949.613	15949.61305	721.4991491
Flowrate	KG-MOL/HR	129.8808794	160.1998897	39.80027322	90.08060615	90.08060615	90.08060666	39.80027322
Total Weight Comp. Rates	KG/HR							
ETHANOL		7.370430123	7363.685207	7.366924313	0.00350585227	0.00350585227	0.003508327745	7.366924313
WATER		715.564997	6.479559975	714.1322241	1.432776988	1.432776988	1.432780939	714.1322241
[EMIM][DCA]		15948.17676	0	7.046369277e-007	15948.17672	15948.17672	15948.17676	7.046369e-007
Total Weight Comp. Fractions								
ETHANOL		0.0004421078834	0.9991208392	0.01021057935	2.198079834e-007	2.198079834e-007	2.199631887e-007	0.01021057935
WATER		0.04292245106	0.000879160803	0.9897894197	8.983145786e-005	8.983145786e-005	8.983170525e-005	0.9897894197
[EMIM][DCA]		0.9566354411	0	9.766289102e-010	0.9999099487	0.9999099487	0.9999099483	9.766289e-010
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		0.1599866283	159.8402195	0.1599105293	7.609996632e-005	7.609996632e-005	7.615370034e-005	0.1599105293
WATER		39.71989367	0.3596702387	39.64036269	0.07953120943	0.07953120943	0.0795314287	39.64036269
[EMIM][DCA]		90.00099908	0	3.976506432e-009	90.00099884	90.00099884	90.00099908	3.97650e-009
Composition								
ETHANOL		0.001231795081	0.9977548659	0.004017824913	8.447985595e-007	8.447985595e-007	8.453950652e-007	0.004017824913
WATER		0.3058178684	0.002245134122	0.995982175	0.0008828893679	0.0008828893679	0.0008828917971	0.995982175
[EMIM][DCA]		0.6929503365	0	9.991153603e-011	0.9991162658	0.9991162658	0.9991162628	9.991153e-011

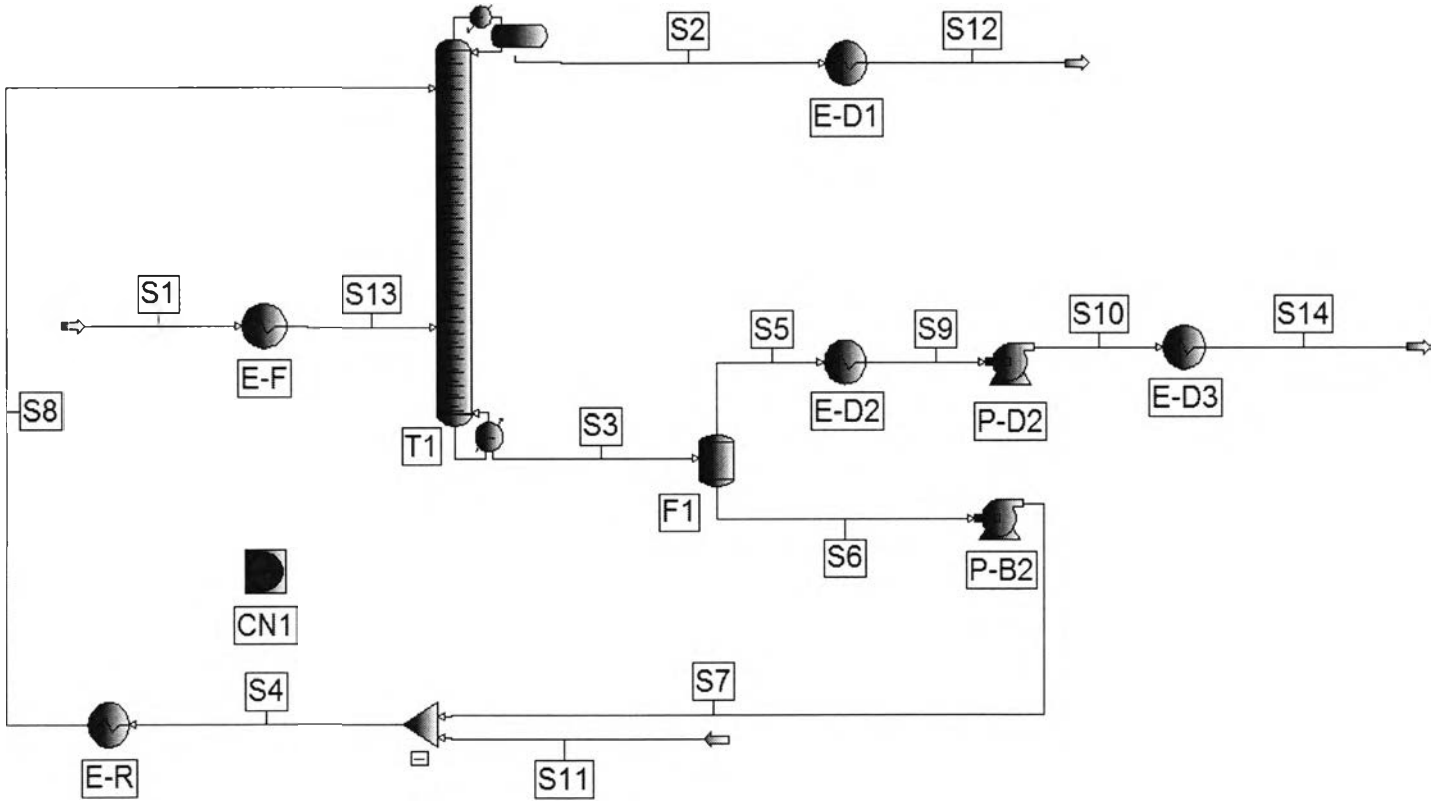

Figure G4 IL process flowsheet using [EMIM][EtSO4] in water + ethanol mixture.

Table G15 Distillation column properties of the IL process using [EMIM][EtSO4] in water + ethanol mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.3917
Reboiler Duty	MM WATT	3.3392
Column Total Molar Feed	KG-MOL/HR	260.0819
Column Total Wt. Feed	KG/HR	22271.5837
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	77.9740
Column Reflux Rate	KG-MOL/HR	154.4829
Column Reflux Ratio		0.9643

Table G16 Flash properties of the IL process using [EMIM][EtSO4] in water + ethanol mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	243.4174
Pressure	KPA	1.0000
DP	KPA	99.0000
Duty	MM WATT	0.7358

Table G17 Pump properties of the IL process using [EMIM][EtSO4] in water + ethanol mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	99.0000	99.0000
Head	M	9.4019	10.1183
Work	HP	0.4867	0.0267

Table G18 Heat exchanger properties of the IL process using [EMIM][EtSO4] in water + ethanol mixture

Hx Name	**Unit**	**E-D1**	**E-F**	**E-R**	**E-D2**
Hx Description					
Duty	MM WATT	0.3434	0.4355	0.1639	0.6152
MTD	C	14.8302	65.4246	110.2041	268.2424

Table G19 Stream table of the IL process using [EMIM][EtSO4] in water + ethanol mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	25	4.725468749	25	30	78	30	77.97398362
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	8091.663905	721.4994732	0.2363000031	7370.164468	8091.663905	721.4994732	7370.164468
Flowrate	KG-MOL/HR	200.0001624	39.80042644	0.001	160.1997364	200.0001624	39.80042644	160.1997364
Total Weight Comp. Rates	KG/HR							
ETHANOL		7371.052129	7.362923504	0	7363.689251	7371.052129	7.362923504	7363.689251
WATER		720.611776	714.1365487	0	6.475216669	720.611776	714.1365487	6.475216669
[EMIM][EtSO4]		0	9.392331722e-007	0.2363000031	0	0	9.392331722e-007	0
Total Weight Comp. Fractions								
ETHANOL		0.9109439314	0.01020502963	0	0.9991214285	0.9109439314	0.01020502963	0.9991214285
WATER		0.08905606863	0.9897949691	0	0.0008785715295	0.08905606863	0.9897949691	0.0008785715295
[EMIM][EtSO4]		0	1.301779429e-009	1	0	0	1.301779429e-009	0
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		160.0001299	0.1598236855	0	159.8403072	160.0001299	0.1598236855	159.8403072
WATER		40.00003248	39.64060275	0	0.3594291486	40.00003248	39.64060275	0.3594291486
[EMIM][EtSO4]		0	3.974748879e-009	0.001	0	0	3.974748879e-009	0
Composition								
ETHANOL		0.8	0.004015627465	0	0.9977563687	0.8	0.004015627465	0.9977563687
WATER		0.2	0.9959843724	0	0.002243631336	0.2	0.9959843724	0.002243631336
[EMIM][EtSO4]		0	9.986699225e-011	1	0	0	9.986699225e-011	0

Table G19 Stream table of the IL process using [EMIM][EtSO4] in water + ethanol mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Vapor	Liquid	Liquid	Liquid	Liquid
Temperature	C	161.1922484	243.5544729	243.4173576	243.4173576	243.5586798	78	4.722209435
Pressure	KPA	100	100	1	1	100	100	1
Total Mass Rate	KG/HR	14901.4192	14179.91976	721.4994732	14179.91973	14179.91973	14179.91976	721.4994732
Flowrate	KG-MOL/HR	99.88220356	60.08177753	39.80042644	60.08177712	60.08177712	60.08177753	39.80042644
Total Weight Comp. Rates	KG/HR							
ETHANOL		7.378765783	0.01588811387	7.362923504	0.01584227631	0.01584227631	0.01588811387	7.362923504
WATER		715.5675536	1.430994249	714.1365487	1.431004683	1.431004683	1.430994249	714.1365487
[EMIM][EtSO4]		14178.47288	14178.47288	9.392331722e-007	14178.47288	14178.47288	14178.47288	9.392331e-007
Total Weight Comp. Fractions								
ETHANOL		0.0004951720158	1.120465711e-006	0.01020502963	1.117233145e-006	1.117233145e-006	1.120465711e-006	0.01020502963
WATER		0.0480200942	0.0001009169497	0.9897949691	0.0001009176858	0.0001009176858	0.0001009169497	0.9897949691
[EMIM][EtSO4]		0.9514847338	0.9998979626	1.301779429e-009	0.9998979651	0.9998979651	0.9998979626	1.301779e-009
Total Molar Comp. Rates	KG-MOL/HR							
ETHANOL		0.1601675668	0.0003448761777	0.1598236855	0.0003438812023	0.0003438812023	0.0003448761777	0.1598236855
WATER		39.72003559	0.07943225237	39.64060275	0.07943283154	0.07943283154	0.07943225237	39.64060275
[EMIM][EtSO4]		60.0020004	60.0020004	3.974748879e-009	60.00200041	60.00200041	60.0020004	3.974748e-009
Composition								
ETHANOL		0.00160356461	5.740112758e-006	0.004015627465	5.723552445e-006	5.723552445e-006	5.740112758e-006	0.004015627465
WATER		0.3976687956	0.001322068947	0.9959843724	0.001322078596	0.001322078596	0.001322068947	0.9959843724
[EMIM][EtSO4]		0.6007276398	0.9986721909	9.986699225e-011	0.9986721979	0.9986721979	0.9986721909	9.986699e-011

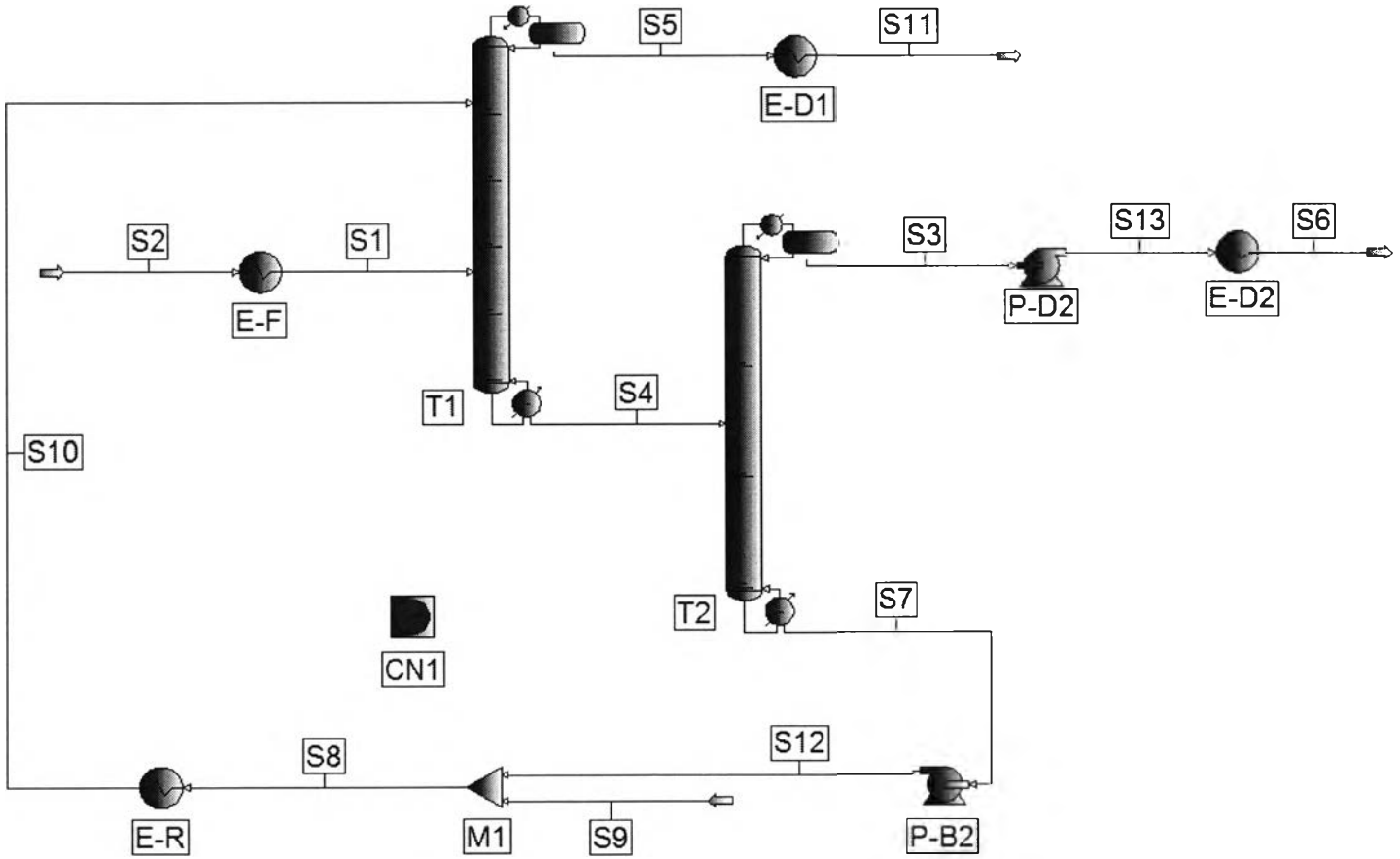

Figure G5 CS process flowsheet using sulfolane in ethanol + hexane mixture.

Table G20 Distillation column properties of the CS process using sulfolane in ethanol + hexane mixture

Column Name	**Unit**	**T1**	**T2**
Column Description			
Condenser Duty	MM WATT	-5.7822	-7.8822
Reboiler Duty	MM WATT	6.4115	27.5645
Column Total Molar Feed	KG-MOL/HR	2499.7204	2199.6180
Column Total Wt. Feed	KG/HR	238315.9591	212481.9714
Column Condenser Pres	KPA	100.0000	75.0000
Column Condenser Temp	C	67.5570	70.6201
Column Reflux Rate	KG-MOL/HR	593.6469	6.4841
Column Reflux Ratio		1.9781	0.0093

Table G21 Pump properties of the CS process using sulfolane in ethanol + hexane mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	25.0000	25.0000
Head	M	2.4404	3.4346
Work	KW	1.1970	0.3020

Table G22 Heat exchanger properties of the CS process using sulfolane in ethanol + hexane mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**
Hx Description					
Duty	MM WATT	19.8355	1.6380	0.6483	1.2705
MTD	C	101.5122	77.2204	11.6533	12.6218

Table G23 Stream table of the CS process using sulfolane in ethanol + hexane mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S2	S3
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	59	59	30	271.5341539	70.62623539	25	70.62012
Pressure	KPA	100	100	100	100	100	100	75
Total Mass Rate	KG/HR	58101.47095	180214.4881	25833.98765	180178.1324	32303.83898	58101.47095	32303.83898
Flowrate	KG-MOL/HR	1000	1499.720412	300.1024206	1499.417881	700.2001113	1000	700.2001113
Total Weight Comp. Rates	KG/HR							
HEXANE		25853.14407	8.669523772e-006	25801.43007	8.671820904e-006	51.7139996	25853.14407	51.7139996
ETHANOL		32248.32687	6.444774026	32.24359796	6.444601903	32216.08345	32248.32687	32216.08345
SULFOLANE		0						
Total Weight Comp. Fractions								
HEXANE		0.4449653968	4.810669699e-011	0.9987397386	4.812915301e-011	0.00160086235	0.4449653968	0.00160086235
ETHANOL		0.5550346032	3.57616865e-005	0.001248107663	3.576794706e-005	0.9972834333	0.5550346032	0.9972834333
SULFOLANE		0	0.9999642383	1.215369148e-005	0.999964232	0.00111570435	0	0.00111570435
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		300	1.006011928e-007	299.3999105	1.006278487e-007	0.6000894837	300	0.6000894837
ETHANOL		700	0.1398938257	0.6998973515	0.1398900895	699.3001064	700	699.3001064
SULFOLANE		0	1499.580519	0.002612734463	1499.27799	0.2999154798	0	0.2999154798
Composition								
HEXANE		0.3	6.707996502e-011	0.9976590989	6.711127701e-011	0.0008570256903	0.3	0.0008570256903
ETHANOL		0.7	9.327993706e-005	0.002332194956	9.329626603e-005	0.9987146461	0.7	0.9987146461
SULFOLANE		0	0.99990672	8.706142583e-006	0.9999067037	0.0004283282378	0	0.0004283282378

Table G23 Stream table of the CS process using sulfolane in ethanol + hexane mixture (Continued)

Stream Name	Unit	S4	S5	S6	S7	S8	S9
Stream Description							
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	88.68530769	67.55698462	30	271.5290442	271.5112915	25
Pressure	KPA	100	100	100	75	100	100
Total Mass Rate	KG/HR	212481.9714	25833.98765	32303.83898	180178.1324	180214.4881	19.55959034
Flowrate	KG-MOL/HR	2199.617992	300.1024206	700.2001113	1499.417881	1499.720412	0.1627628827
Total Weight Comp. Rates	KG/HR						
HEXANE		51.71400827	25801.43007	51.7139996	8.671820904e-006	8.669523772e-006	0
ETHANOL		32222.52805	32.24359796	32216.08345	6.444601903	6.444774026	0
SULFOLANE		180207.7293					
Total Weight Comp. Fractions							
HEXANE		0.0002433806875	0.9987397386	0.00160086235	4.812915301e-011	4.810669699e-011	0
ETHANOL		0.151648292	0.001248107663	0.9972834333	3.576794706e-005	3.57616865e-005	0
SULFOLANE		0.8481083273	1.215369148e-005	0.00111570435	0.999964232	0.9999642383	1
Total Molar Comp. Rates	KG-MOL/HR						
HEXANE		0.6000895844	299.3999105	0.6000894837	1.006278487e-007	1.006011928e-007	0
ETHANOL		699.4399965	0.6998973515	699.3001064	0.1398900895	0.1398938257	0
SULFOLANE		1499.577906	0.002612734463	0.2999154798	1499.27799	1499.580519	0.1627628827
Composition							
HEXANE		0.0002728153646	0.9976590989	0.0008570256903	6.711127701e-011	6.707996502e-011	0
ETHANOL		0.3179824856	0.002332194956	0.9987146461	9.329626603e-005	9.327993706e-005	0
SULFOLANE		0.681744699	8.706142583e-006	0.0004283282378	0.9999067037	0.99990672	1

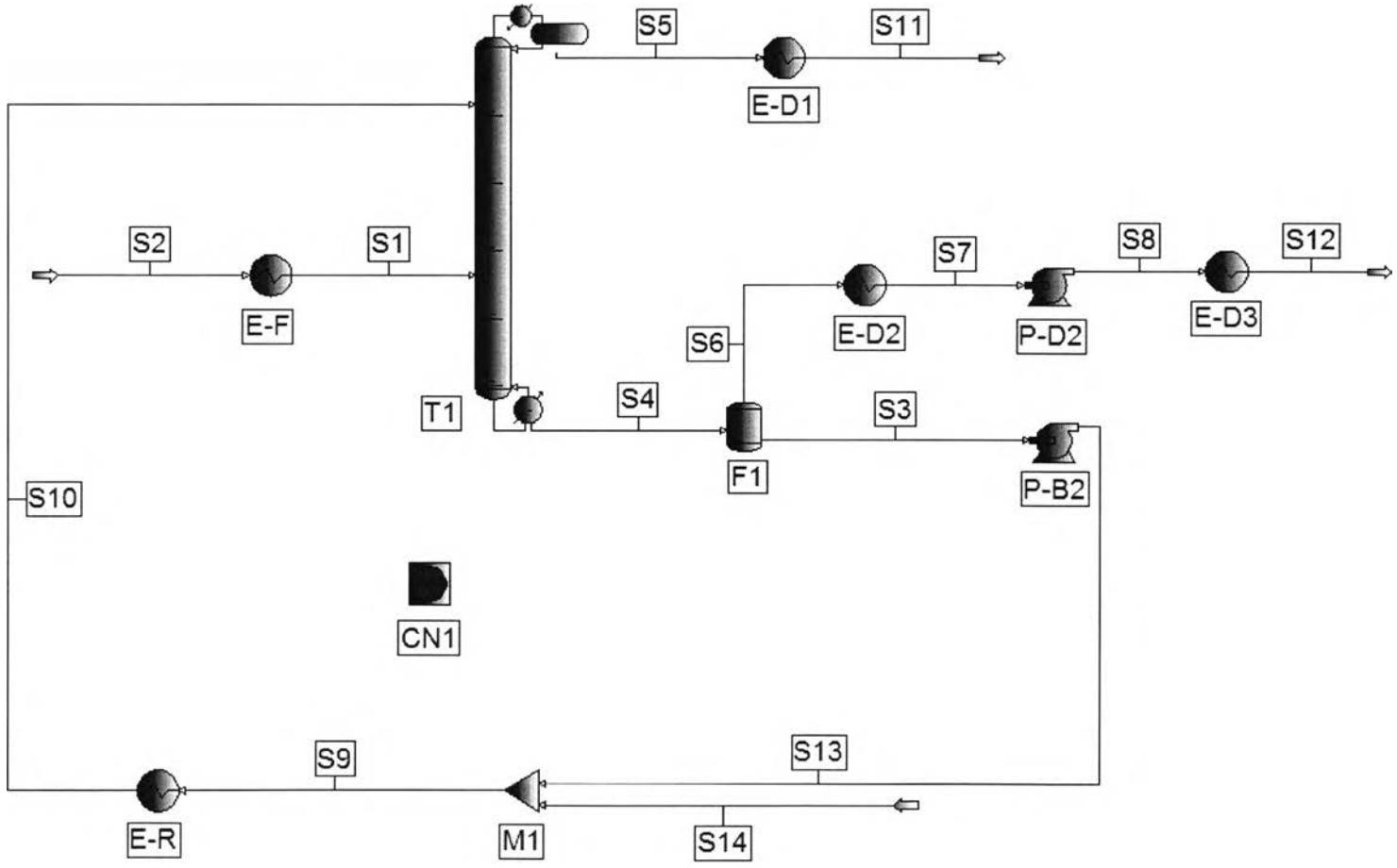

Figure G6 IL process flowsheet using [EMIM][BTI] in ethanol + hexane mixture.

Table G24 Distillation column properties of the IL process using [EMIM][BTI] in ethanol + hexane mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-13.5849
Reboiler Duty	MM WATT	6.4023
Column Total Molar Feed	KG-MOL/HR	2100.0652
Column Total Wt. Feed	KG/HR	488544.8190
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	68.2679
Column Reflux Rate	KG-MOL/HR	1754.2934
Column Reflux Ratio		5.8477

Table G25 Flash properties of the IL process using [EMIM][BTI] in ethanol + hexane mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	216.1716
Pressure	KPA	0.1000
DP	KPA	99.9000
Duty	MM WATT	19.6996

Table G26 Pump properties of the IL process using [EMIM][BTI] in ethanol + hexane mixture

Pump Name	**Unit**	**P-D2**	**P-B2**
Pump Description			
Pressure Gain	KPA	99.9000	99.9000
Head	M	12.2110	7.6931
Work	KW	1.0728	9.0145

Table G27 Heat exchanger properties of the IL process using [EMIM][BTI] in ethanol + hexane mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	1.9460	1.6380	0.6609	13.2858	1.9284
MTD	C	84.9326	77.2204	11.8805	230.7471	1119.5

Table G28 Stream table of the IL process using [EMIM][BTI] in ethanol + hexane mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	59	59	30	30	216.3820755	25	25
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	58101.47095	430443.348	25828.86022	32272.61096	430443.348	3.912999878	58101.47095
Flowrate	KG-MOL/HR	1000	1100.06522	299.9952404	700.0047595	1100.065221	0.01	1000
Total Weight Comp. Rates	KG/HR							
HEXANE		25853.14407	0.0001681274826	25801.4384	51.70567828	0.0001681288048	0	25853.14407
ETHANOL		32248.32687	1.622505798	27.42182718	32220.90501	1.622520549	0	32248.32687
[EMIM][BTI]		0	430441.7254	7.67776e-008	0.0002739030833	430441.7253	3.912999878	0
Total Weight Comp. Fractions								
HEXANE		0.4449653968	3.905914294e-010	0.9989383261	0.001602153552	3.905945013e-010	0	0.4449653968
ETHANOL		0.5550346032	3.769382906e-006	0.00106167	0.998397838	3.769417176e-006	0	0.5550346032
[EMIM][BTI]		0	0.9999962302	2.97255e-012	8.48716838e-009	0.9999962302	1	0
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		300	1.950952063e-006	299.4000071	0.5999929231	1.950967407e-006	0	300
ETHANOL		700	0.03521900727	0.5952333311	699.4047658	0.03521932746	0	700
[EMIM][BTI]		0	1100.029999	1.962117e-010	6.999823456e-007	1100.029999	0.01	0
Composition								
HEXANE		0.3	1.773487632e-009	0.9980158574	0.0008571269195	1.77350158e-009	0	0.3
ETHANOL		0.7	3.20153811e-005	0.0019841425	0.9991428721	3.201567217e-005	0	0.7
[EMIM][BTI]		0	0.9999679828	6.540494e-013	9.999679804e-010	0.9999679826	1	0

Table G28 Stream table of the IL process using [EMIM][BTI] in ethanol + hexane mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid
Temperature	C	216.1716423	109.3659377	68.2678966	216.1716423	-33.71860842	-33.70749118	216.3807864
Pressure	KPA	0.1	100	100	0.1	0.1	100	100
Total Mass Rate	KG/HR	430443.348	462715.9587	25828.86022	32272.61096	32272.61096	32272.61096	430443.348
Flowrate	KG-MOL/HR	1100.065221	1800.06998	299.9952404	700.0047595	700.0047595	700.0047595	1100.06522
Total Weight Comp. Rates	KG/HR							
HEXANE		0.0001681288048	51.70584645	25801.4384	51.70567828	51.70567828	51.70567828	0.0001681274826
ETHANOL		1.622520549	32222.52755	27.42182718	32220.90501	32220.90501	32220.90501	1.622505798
[EMIM][BTI]		430441.7253	430441.7254	7.677764101e-008	0.0002739030833	0.0002739030833	0.0002739030833	430441.7254
Total Weight Comp. Fractions								
HEXANE		3.905945013e-010	0.0001117442471	0.9989383261	0.001602153552	0.001602153552	0.001602153552	3.905914e-010
ETHANOL		3.769417176e-006	0.06963781331	0.001061673916	0.998397838	0.998397838	0.998397838	3.7693829e-006
[EMIM][BTI]		0.9999962302	0.9302504424	2.972552422e-012	8.48716838e-009	8.48716838e-009	8.48716838e-009	0.9999962302
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		1.950967407e-006	0.5999948745	299.4000071	0.5999929231	0.5999929231	0.5999929231	1.950952e-006
ETHANOL		0.03521932746	699.4399857	0.5952333311	699.4047658	699.4047658	699.4047658	0.03521900727
[EMIM][BTI]		1100.029999	1100.029999	1.962117133e-010	6.999823456e-007	6.999823456e-007	6.999823456e-007	1100.029999
Composition								
HEXANE		1.77350158e-009	0.0003333175272	0.9980158574	0.0008571269195	0.0008571269195	0.0008571269195	1.7734876e-009
ETHANOL		3.201567217e-005	0.3885626634	0.001984142583	0.9991428721	0.9991428721	0.9991428721	3.20153811e-005
[EMIM][BTI]		0.9999679826	0.6111040191	6.54049421e-013	9.999679804e-010	9.999679804e-010	9.999679804e-010	0.9999679828

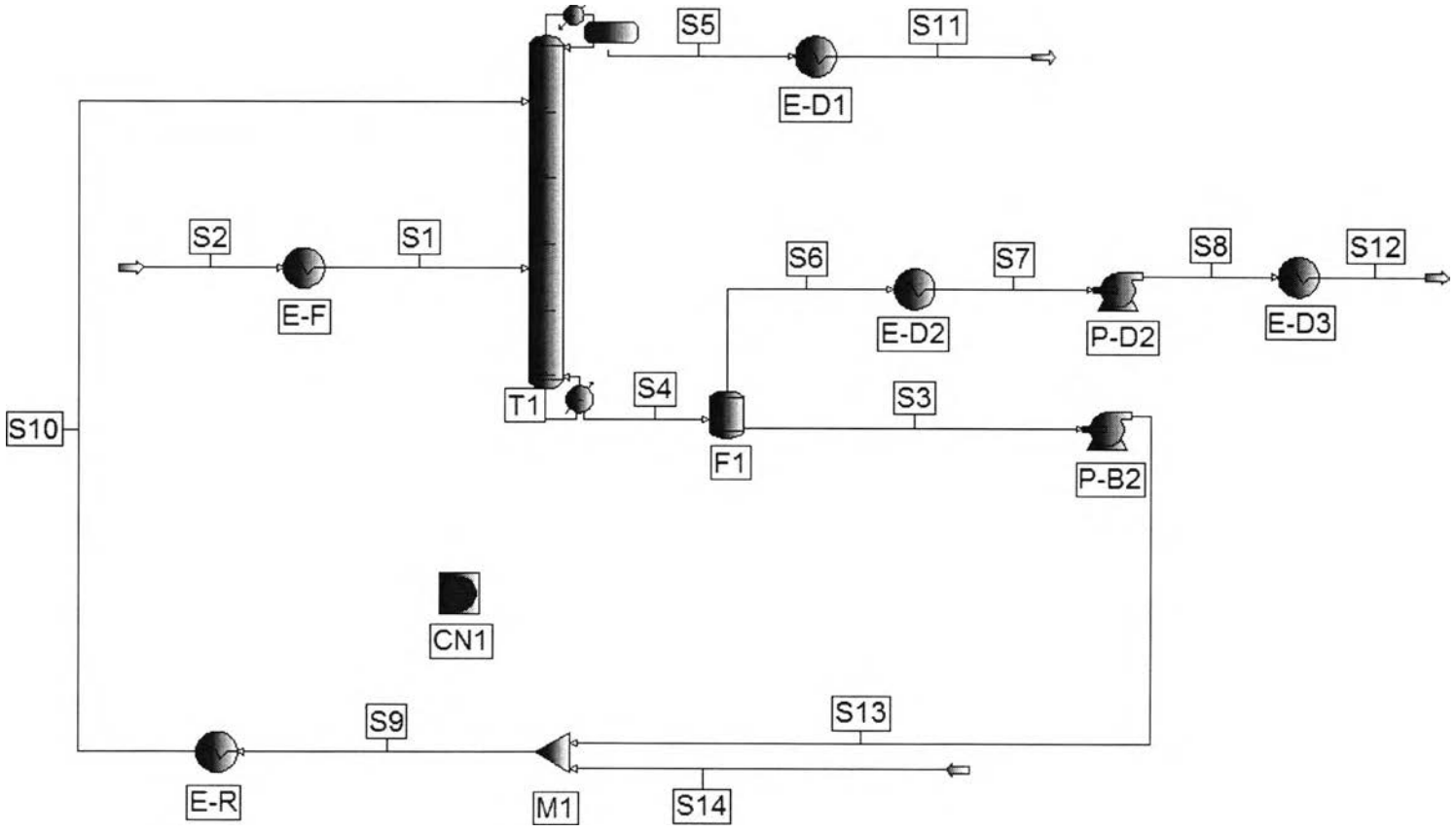

Figure G7 IL process flowsheet using [BMIM][BTI] in ethanol + hexane mixture.

Table G29 Distillation column properties of the IL process using [BMIM][BTI] in ethanol + hexane mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-15.0016
Reboiler Duty	MM WATT	8.4693
Column Total Molar Feed	KG-MOL/HR	2100.0859
Column Total Wt. Feed	KG/HR	519464.0889
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	68.2796
Column Reflux Rate	KG-MOL/HR	1751.4048
Column Reflux Ratio		5.8381

Table G30 Flash properties of the IL process using [BMIM][BTI] in ethanol + hexane mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	243.7095
Pressure	KPA	0.1000
DP	KPA	99.9000
Duty	MM WATT	20.3206

Table G31 Pump properties of the IL process using [BMIM][BTI] in ethanol + hexane mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	99.9000	99.9000
Head	M	8.4841	12.2103
Work	KW	10.6553	1.0727

Table G32 Heat exchanger properties of the IL process using [BMIM][BTI] in ethanol + hexane mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	2.7021	1.6380	0.6611	13.8038	1.93
MTD	C	93.3547	77.2204	11.8842	240.5061	119.5242

Table G33 Stream table of the IL using [BMIM][BTI] in ethanol + hexane mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	59	59	30	30	243.9118934	25	25
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	58101.47095	461362.618	25828.89005	32272.58113	461362.6181	4.193999939	58101.47095
Flowrate	KG-MOL/HR	1000	1100.085889	299.9958887	700.0041107	1100.08589	0.01	1000
Total Weight Comp. Rates	KG/HR							
HEXANE		25853.14407	0.0002711780811	25801.43832	51.70575272	0.0002711756319	0	25853.14407
ETHANOL		32248.32687	1.653088307	27.45173303	32220.87508	1.653103361	0	32248.32687
[BMIM][BTI]		0	461360.9646	9.196777e-008	0.0002935721417	461360.9648	4.193999939	0
Total Weight Comp. Fractions								
HEXANE		0.4449653968	5.877764485e-010	0.9989371695	0.00160215734	5.877711398e-010	0	0.4449653968
ETHANOL		0.5550346032	3.583056456e-006	0.0010628305	0.9983978336	3.583089084e-006	0	0.5550346032
[BMIM][BTI]		0	0.9999964164	3.560655e-012	9.096642769e-009	0.9999964163	1	0
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		300	3.146751671e-006	299.4000062	0.599993787	3.146723251e-006	0	300
ETHANOL		700	0.03588284811	0.5958824839	699.4041162	0.03588317487	0	700
[BMIM][BTI]		0	1100.050003	2.192841e-010	6.999812733e-007	1100.050003	0.01	0
Composition								
HEXANE		0.3	2.86045999e-009	0.9980136978	0.000857128948	2.860434154e-009	0	0.3
ETHANOL		0.7	3.261822414e-005	0.001986302	0.9991428701	3.261852116e-005	0	0.7
[BMIM][BTI]		0	0.9999673789	7.30957e-013	9.999673754e-010	0.9999673786	1	0

Table G33 Stream table of the IL process using [BMIM][BTI] in ethanol + hexane mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid
Temperature	C	243.7094909	123.6896304	68.27955587	243.7094909	-33.77416585	-33.76305513	243.9107715
Pressure	KPA	0.1	100	100	0.1	0.1	100	100
Total Mass Rate	KG/HR	461362.6181	493635.1989	25828.89005	32272.58113	32272.58113	32272.58113	461362.618
Flowrate	KG-MOL/HR	1100.08589	1800.09	299.9958887	700.0041107	700.0041107	700.0041107	1100.085889
Total Weight Comp. Rates	KG/HR							
HEXANE		0.0002711756319	51.70602398	25801.43832	51.70575272	51.70575272	51.70575272	0.0002711780811
ETHANOL		1.653103361	32222.52823	27.45173303	32220.87508	32220.87508	32220.87508	1.653088307
[BMIM][BTI]		461360.9648	461360.9646	9.196777784e-008	0.0002935721417	0.0002935721417	0.0002935721417	461360.9646
Total Weight Comp. Fractions								
HEXANE		5.877711398e-010	0.0001047454154	0.9989371695	0.00160215734	0.00160215734	0.00160215734	5.8777644e-010
ETHANOL		3.583089084e-006	0.0652759939	0.001062830535	0.9983978336	0.9983978336	0.9983978336	3.583056e-006
[BMIM][BTI]		0.9999964163	0.9346192607	3.560655439e-012	9.096642769e-009	9.096642769e-009	9.096642769e-009	0.9999964164
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		3.146723251e-006	0.5999969346	299.4000062	0.599993787	0.599993787	0.599993787	3.1467516e-006
ETHANOL		0.03588317487	699.4400004	0.5958824839	699.4041162	699.4041162	699.4041162	0.03588284811
[BMIM][BTI]		1100.050003	1100.050003	2.192841659e-010	6.999812733e-007	6.999812733e-007	6.999812733e-007	1100.050003
Composition								
HEXANE		2.860434154e-009	0.0003333149645	0.9980136978	0.000857128948	0.000857128948	0.000857128948	2.86045999e-009
ETHANOL		3.261852116e-005	0.38855835	0.001986302167	0.9991428701	0.9991428701	0.9991428701	3.2618224e-005
[BMIM][BTI]		0.9999673786	0.6111083351	7.30957237e-013	9.999673754e-010	9.999673754e-010	9.999673754e-010	0.9999673789

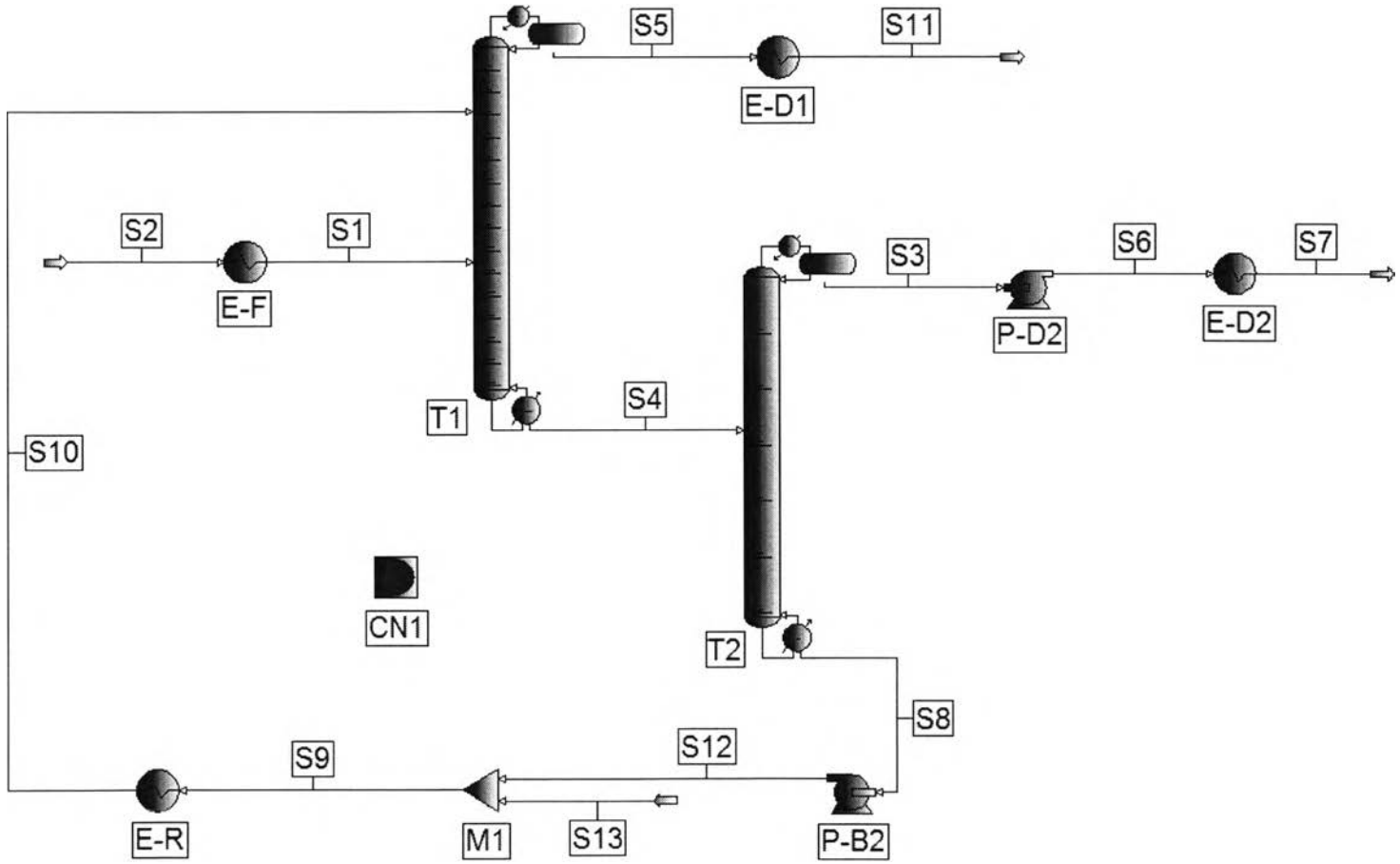

Figure G8 CS process flowsheet using NMP in benzene + hexane mixture.

Table G34 Distillation column properties of the CS process using NMP in benzene + hexane mixture

Column Name	**Unit**	**T1**	**T2**
Column Description			
Condenser Duty	MM WATT	-4.2285	-8.0086
Reboiler Duty	MM WATT	8.9710	8.1283
Column Total Molar Feed	KG-MOL/HR	2300.1090	1999.3923
Column Total Wt. Feed	KG/HR	209411.1137	183496.6070
Column Condenser Pres	KPA	100.0000	20.0000
Column Condenser Temp	C	68.3444	35.3233
Column Reflux Rate	KG-MOL/HR	224.6653	175.0000
Column Reflux Ratio		0.7471	0.2500

Table G35 Pump properties of the separation process using NMP in benzene + hexane mixture

Pump Name	**Unit**	**P-D2**	**P-B2**
Pump Description			
Pressure Gain	KPA	80.0000	80.0000
Head	M	9.4649	8.8500
Work	KW	1.4091	3.1032

Table G36 Heat exchanger properties of the separation process using NMP in benzene + hexane mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**
Hx Description					
Duty	MM WATT	5.7609	1.8836	0.6635	0.1377
MTD	C	68.2188	71.8316	11.9048	5.1704

Table G37 Stream table of the CS process using NMP in benzene + hexane mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S2	S3
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	68	68	30	146.8303084	25	25	35.32327425
Pressure	KPA	100	100	100	100	100	100	20
Total Mass Rate	KG/HR	80532.69196	128878.4218	25914.50672	128807.388	65.15777772	80532.69196	54689.219
Flowrate	KG-MOL/HR	1000	1300.109042	300.7167213	1299.392303	0.6572790734	1000	700.0000173
Total Weight Comp. Rates	KG/HR							
HEXANE		25853.14407	8.057048897e-007	25827.28856	8.023674348e-007	0	25853.14407	25.8555146
BENZENE		54679.54788	17.67650523	50.44857962	17.60839221	0	54679.54788	54629.16769
NMP		0						
Total Weight Comp. Fractions								
HEXANE		0.3210266967	6.251666326e-012	0.9966343887	6.229203523e-012	0	0.3210266967	0.000472771692
BENZENE		0.6789733033	0.0001371564377	0.001946731233	0.0001367032784	0	0.6789733033	0.9989019534
NMP		0	0.9998628436	0.001418880049	0.9998632967	1	0	0.0006252748679
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		300	9.34940316e-009	299.6999725	9.310675319e-009	0	300	0.3000275076
BENZENE		700	0.2262921722	0.6458357302	0.2254201987	0	700	699.3550397
NMP		0	1299.88275	0.3709130984	1299.166883	0.6572790734	0	0.344950069
Composition								
HEXANE		0.3	7.191245395e-012	0.9966189149	7.165407473e-012	0	0.3	0.0004286107146
BENZENE		0.7	0.0001740563021	0.002147654867	0.0001734812483	0	0.7	0.9990786035
NMP		0	0.9998259437	0.001233430242	0.9998265187	1	0	0.0004927858006

Table G37 Stream table of the conventional extractive distillation process using NMP in benzene + hexane mixture (Continued)

Stream Name	Unit	S4	S5	S6	S7	S8	S9
Stream Description							
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	111.8325486	68.34441426	35.34463577	30	146.8139517	146.7747058
Pressure	KPA	100	100	100	100	20	100
Total Mass Rate	KG/HR	183496.607	25914.50672	54689.219	54689.219	128807.388	128878.4218
Flowrate	KG-MOL/HR	1999.39232	300.7167213	700.0000173	700.0000173	1299.392303	1300.109042
Total Weight Comp. Rates	KG/HR						
HEXANE		25.85551516	25827.28856	25.8555146	25.8555146	8.023674348e-007	8.057048897e-007
BENZENE		54646.77581	50.44857962	54629.16769	54629.16769	17.60839221	17.67650523
NMP		128823.9757					
Total Weight Comp. Fractions							
HEXANE		0.0001409045953	0.9966343887	0.000472771692	0.000472771692	6.229203523e-012	6.251666326e-012
BENZENE		0.2978080995	0.001946731233	0.9989019534	0.9989019534	0.0001367032784	0.0001371564377
NMP		0.7020509959	0.001418880049	0.0006252748679	0.0006252748679	0.9998632967	0.9998628436
Total Molar Comp. Rates	KG-MOL/HR						
HEXANE		0.3000275141	299.6999725	0.3000275076	0.3000275076	9.310675319e-009	9.34940316e-009
BENZENE		699.5804564	0.6458357302	699.3550397	699.3550397	0.2254201987	0.2262921722
NMP		1299.511836	0.3709130984	0.344950069	0.344950069	1299.166883	1299.88275
Composition							
HEXANE		0.000150059351	0.9966189149	0.0004286107146	0.0004286107146	7.165407473e-012	7.191245395e-012
BENZENE		0.3498965407	0.002147654867	0.9990786035	0.9990786035	0.0001734812483	0.0001740563021
NMP		0.6499533999	0.001233430242	0.0004927858006	0.0004927858006	0.9998265187	0.9998259437

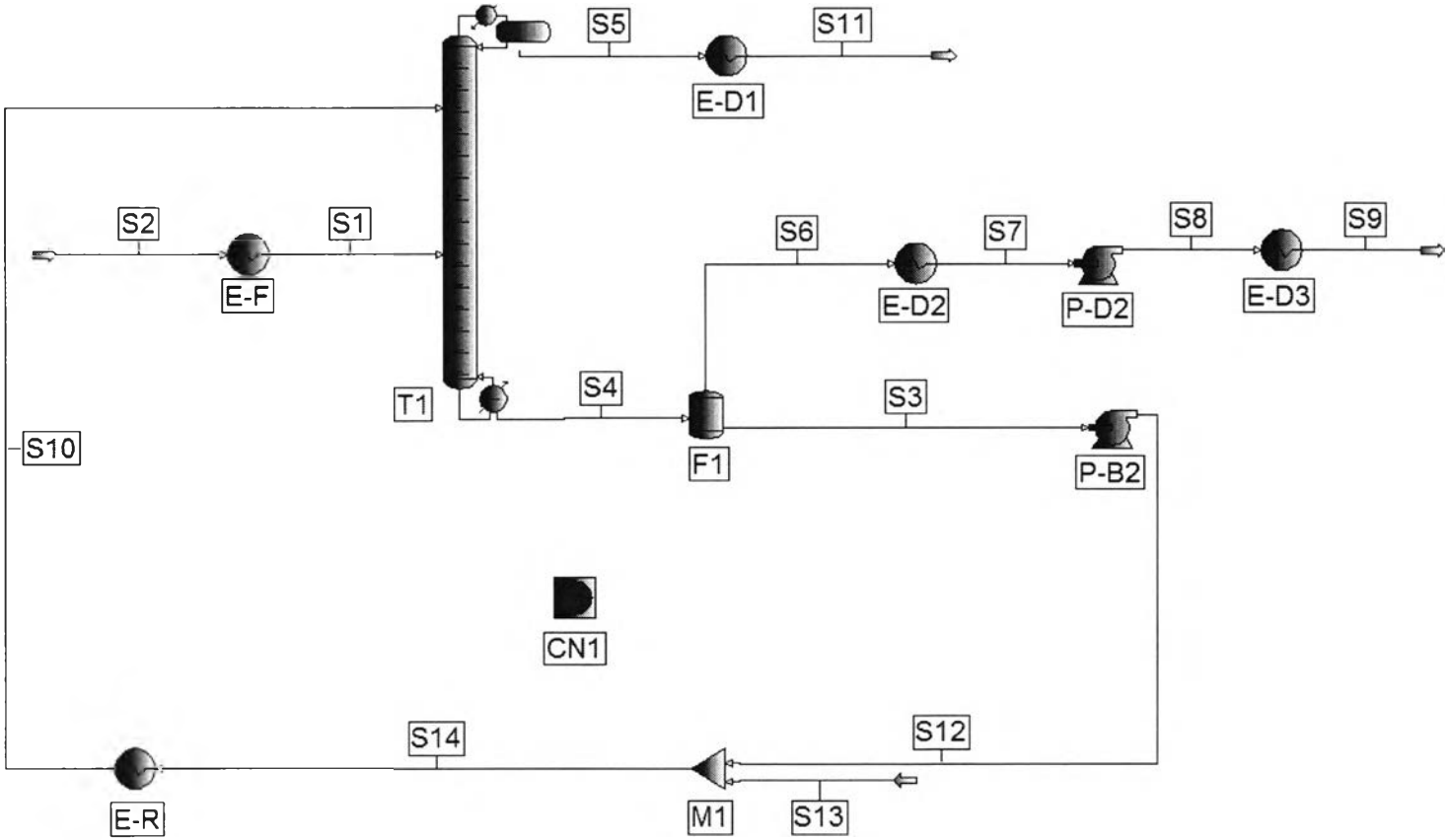

Figure G9 IL process flowsheet using [EMIM][EtSO4] in benzene + hexane mixture.

Table G38 Distillation column properties of the IL process using [EMIM][EtSO4] in benzene + hexane mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-3.3015
Reboiler Duty	MM WATT	3.4210
Column Total Molar Feed	KG-MOL/HR	1400.3407
Column Total Wt. Feed	KG/HR	175110.9475
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	68.3137
Column Reflux Rate	KG-MOL/HR	110.3250
Column Reflux Ratio		0.3672

Table G39 Flash properties of the IL process using [EMIM][EtSO4] in benzene + hexane mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	80.3026
Pressure	KPA	0.1000
DP	KPA	99.9000
Duty	MM WATT	6.2482

Table G40 Pump properties of the IL process using [EMIM][EtSO4] in benzene + hexane mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	99.9000	99.9000
Head	M	8.1915	10.7650
Work	KW	2.1090	1.6014

Table G41 Heat exchanger properties of the IL process using [EMIM][EtSO4] in benzene + hexane mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	0.0694	1.8836	0.6625	9.1892	1.8537
MTD	C	39.0584	71.8316	11.8951	167.7354	126.7206

Table G42 Stream table of the IL process using [EMIM][EtSO4] in benzene + hexane mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	68	68	30	80.37895085	25	80.36541168	25
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	80532.69196	94578.25557	25887.49151	94578.25849	23.63000031	94578.25557	80532.69196
Flowrate	KG-MOL/HR	1000	400.3407032	300.4706799	400.3407392	0.1	400.3407032	1000
Total Weight Comp. Rates	KG/HR							
HEXANE		25853.14407	0.0001146241618	25827.29066	0.0001146538702	0	0.0001146241618	25853.14407
BENZENE		54679.54788	10.98901052	60.2008506	10.99176156	0	10.98901052	54679.54788
[EMIM][EtSO4]		0	94567.26644	2.007315e-010	94567.26661	23.63000031	94567.26644	0
Total Weight Comp. Fractions								
HEXANE		0.3210266967	1.211950476e-009	0.9976745197	1.212264552e-009	0	1.211950476e-009	0.3210266967
BENZENE		0.6789733033	0.0001161896089	0.0023254802	0.0001162186928	0	0.0001161896089	0.6789733033
[EMIM][EtSO4]		0	0.9998838092	7.753999e-015	0.9998837801	1	0.9998838092	0
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		300	1.330099289e-006	299.6999969	1.330444025e-006	0	1.330099289e-006	300
BENZENE		700	0.140679791	0.7706829528	0.1407150094	0	0.140679791	700
[EMIM][EtSO4]		0	400.2000221	8.494777e-013	400.2000228	0.1	400.2000221	0
Composition								
HEXANE		0.3	3.322418326e-009	0.997435081	3.323279133e-009	0	3.322418326e-009	0.3
BENZENE		0.7	0.0003514001695	0.00256491899	0.0003514881091	0	0.0003514001695	0.7
[EMIM][EtSO4]		0	0.9996485965	2.827156e-015	0.9996485086	1	0.9996485965	0

Table G42 Stream table of the IL process using [EMIM][EtSO4] in benzene + hexane mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Liquid	Liquid	Liquid	Vapor	Liquid	Liquid	Liquid
Temperature	C	80.30263356	76.27390643	68.31371447	80.30263356	-51.1280891	-51.10681849	30
Pressure	KPA	0.1	100	100	0.1	0.1	100	100
Total Mass Rate	KG/HR	94578.25849	149223.456	25887.49151	54645.19774	54645.19774	54645.19774	54645.19774
Flowrate	KG-MOL/HR	400.3407392	1099.870023	300.4706799	699.5292842	699.5292842	699.5292842	699.5292842
Total Weight Comp. Rates	KG/HR							
HEXANE		0.0001146538702	25.85352391	25827.29066	25.8534092	25.8534092	25.8534092	25.8534092
BENZENE		10.99176156	54630.33604	60.2008506	54619.34417	54619.34417	54619.34417	54619.34417
[EMIM][EtSO4]		94567.26661	94567.26644	2.007315879e-010	0.0001652406669	0.0001652406669	0.0001652406669	0.0001652406669
Total Weight Comp. Fractions								
HEXANE		1.212264552e-009	0.0001732537538	0.9976745197	0.0004731140204	0.0004731140204	0.0004731140204	0.0004731140204
BENZENE		0.0001162186928	0.3660975124	0.002325480264	0.999526883	0.999526883	0.999526883	0.999526883
[EMIM][EtSO4]		0.9998837801	0.6337292338	7.753999175e-015	3.023882678e-009	3.023882678e-009	3.023882678e-009	3.023882e-009
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		1.330444025e-006	0.3000044076	299.6999969	0.3000030765	0.3000030765	0.3000030765	0.3000030765
BENZENE		0.1407150094	699.3699968	0.7706829528	699.2292804	699.2292804	699.2292804	699.2292804
[EMIM][EtSO4]		400.2000228	400.2000221	8.494777201e-013	6.992833887e-007	6.992833887e-007	6.992833887e-007	6.9928338e-007
Composition								
HEXANE		3.323279133e-009	0.0002727635095	0.997435081	0.0004288642138	0.0004288642138	0.0004288642138	0.0004288642138
BENZENE		0.0003514881091	0.6358660405	0.00256491899	0.9995711348	0.9995711348	0.9995711348	0.9995711348
[EMIM][EtSO4]		0.9996485086	0.363861196	2.827156781e-015	9.996484845e-010	9.996484845e-010	9.996484845e-010	9.996484e-010

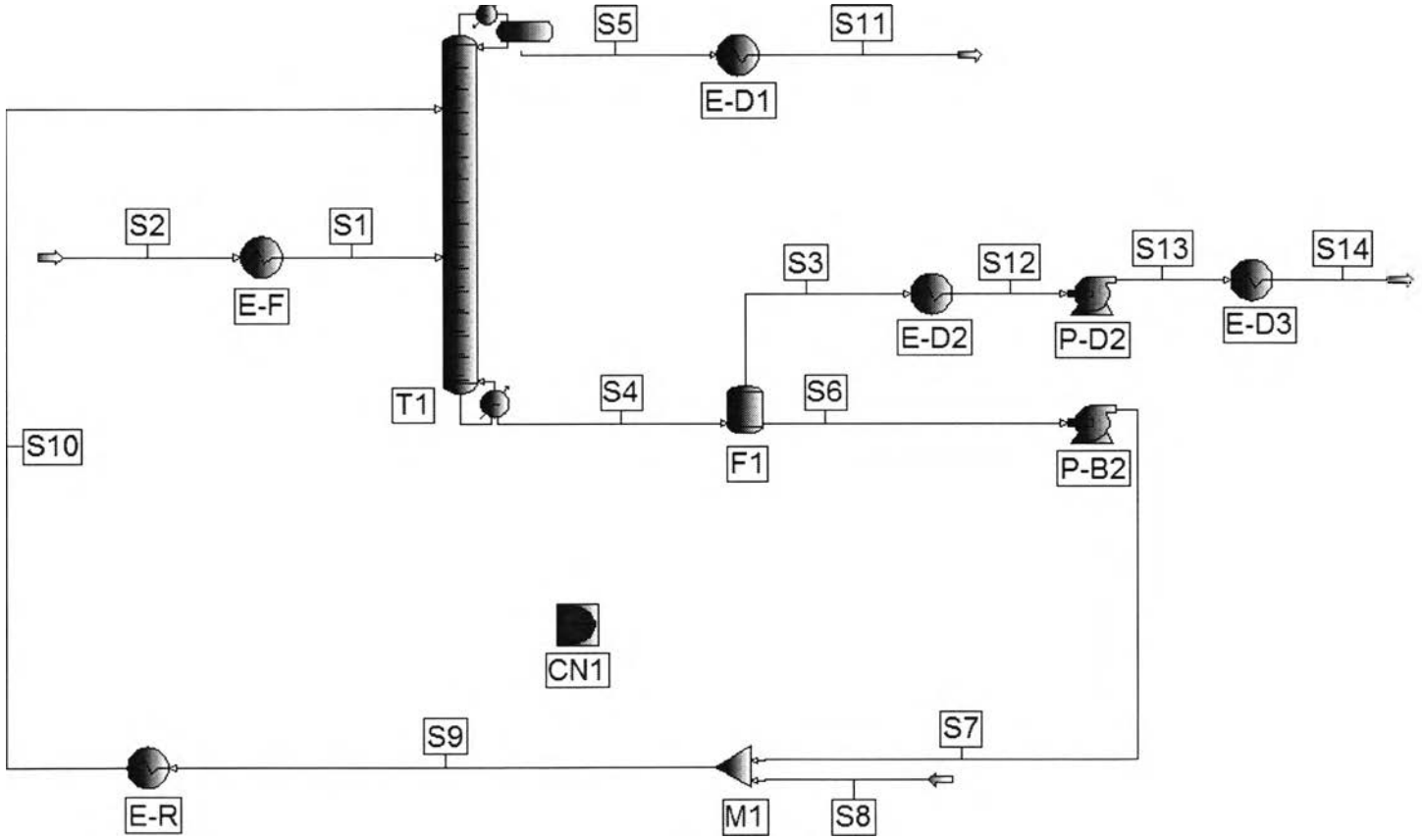

Figure G10 IL process flowsheet using [BMIM][BTI] in benzene + hexane mixture.

Table G43 Distillation column properties of the IL process using [BMIM][BTI] in benzene + hexane mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-5.8069
Reboiler Duty	MM WATT	4.4768
Column Total Molar Feed	KG-MOL/HR	1600.1379
Column Total Wt. Feed	KG/HR	332183.4631
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	68.3137
Column Reflux Rate	KG-MOL/HR	422.0705
Column Reflux Ratio		1.4047

Table G44 Flash properties of the IL process using [BMIM][BTI] in benzene + hexane mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	119.7857
Pressure	KPA	0.1000
DP	KPA	99.9000
Duty	MM WATT	8.8363

Table G45 Pump properties of the IL process using [BMIM][BTI] in benzene + hexane mixture

Pump Name	**Unit**	**P-D2**	**P-B2**
Pump Description			
Pressure Gain	KPA	99.9000	99.9000
Head	M	10.7650	7.6910
Work	KW	1.6014	5.2687

Table G46 Heat exchanger properties of the IL process using [BMIM][BTI] in benzene + hexane mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	0.3952	1.8836	0.6625	10.0051	1.8537
MTD	C	0.0100	71.8316	11.8951	182.8492	128.7206

Table G47 Stream table of IL-based separation process using [BMIM][BTI] in benzene + hexane mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	68	68	30	-51.12808835	-51.10681773	30	25
Pressure	KPA	100	100	100	0.1	100	100	100
Total Mass Rate	KG/HR	80532.69196	251650.7712	25887.23727	54645.45578	54645.45578	54645.45578	80532.69196
Flowrate	KG-MOL/HR	1000	600.1379373	300.4674239	699.532587	699.532587	699.532587	1000
HEXANE		25853.14407	0.000390162971	25827.29164	25.85243743	25.85243743	25.85243743	25853.14407
BENZENE		54679.54788	10.77442854	59.94563348	54619.60305	54619.60305	54619.60305	54679.54788
[BMIM][BTI]		0	251639.9963	0	0.0002933165353	0.0002933165353	0.0002933165353	0
Total Weight Comp. Fractions								
HEXANE		0.3210266967	1.550414367e-009	0.9976843557	0.0004730940033	0.0004730940033	0.0004730940033	0.3210266967
BENZENE		0.6789733033	4.281500308e-005	0.0023156443	0.9995269006	0.9995269006	0.9995269006	0.6789733033
[BMIM][BTI]		0	0.9999571834	0	5.367629039e-009	5.367629039e-009	5.367629039e-009	0
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		300	4.527452869e-006	299.7000082	0.2999918002	0.2999918002	0.2999918002	300
BENZENE		700	0.1379327422	0.7674156985	699.2325945	699.2325945	699.2325945	700
[BMIM][BTI]		0	600	0	6.993718158e-007	6.993718158e-007	6.993718158e-007	0
Composition								
HEXANE		0.3	7.544020445e-009	0.9974459271	0.0004288460691	0.0004288460691	0.0004288460691	0.3
BENZENE		0.7	0.0002298350656	0.0025540728	0.9995711529	0.9995711529	0.9995711529	0.7
[BMIM][BTI]		0	0.9997701574	0	9.997701733e-010	9.997701733e-010	9.997701733e-010	0

Table G47 Stream table of IL-based separation process using [BMIM][BTI] in benzene + hexane mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	119.7857468	88.25257994	68.31371016	119.7857468	119.9073999	25	119.9054173
Pressure	KPA	0.1	100	100	0.1	100	100	100
Total Mass Rate	KG/HR	54645.45578	306296.2258	25887.23727	251650.7691	251650.7691	0.00151572452	251650.7712
Flowrate	KG-MOL/HR	699.532587	1299.670513	300.4674239	600.1379263	600.1379263	3.61403e-006	600.1379373
Total Weight Comp. Rates	KG/HR							
HEXANE		25.85243743	25.85282767	25827.29164	0.000390340526	0.000390340526	0	0.000390162971
BENZENE		54619.60305	54630.37668	59.94563348	10.77385725	10.77385725	0	10.77442854
[BMIM][BTI]		0.0002933165353	251639.9963	0	251639.9948	251639.9948	0.00151572452	251639.9963
Total Weight Comp. Fractions								
HEXANE		0.0004730940033	8.4404653e-005	0.9976843557	1.5511199e-009	1.5511199e-009	0	1.550414e-009
BENZENE		0.9995269006	0.1783579818	0.002315644302	4.2812733e-005	4.281273e-005	0	4.281500e-005
[BMIM][BTI]		5.367629039e-009	0.8215576135	0	0.9999571857	0.9999571857	1	0.9999571834
Total Molar Comp. Rates	KG-MOL/HR							
HEXANE		0.2999918002	0.2999963284	299.7000082	4.5295132e-006	4.5295132e-006	0	4.527452e-006
BENZENE		699.2325945	699.370517	0.7674156985	0.1379254286	0.1379254286	0	0.1379327422
[BMIM][BTI]		6.993718158e-007	600	0	599.9999964	599.9999964	3.614030859e-006	600
Composition								
HEXANE		0.00042884606	0.00023082490	0.9974459271	7.547453708e-009	7.54745370e-009	0	7.544020e-009
BENZENE		0.9995711529	0.5381137064	0.002554072	0.0002298228	0.0002298228	0	0.00022983506
[BMIM][BTI]		9.99770173e-010	0.4616554687	0	0.9997701696	0.9997701696	1	0.9997701574

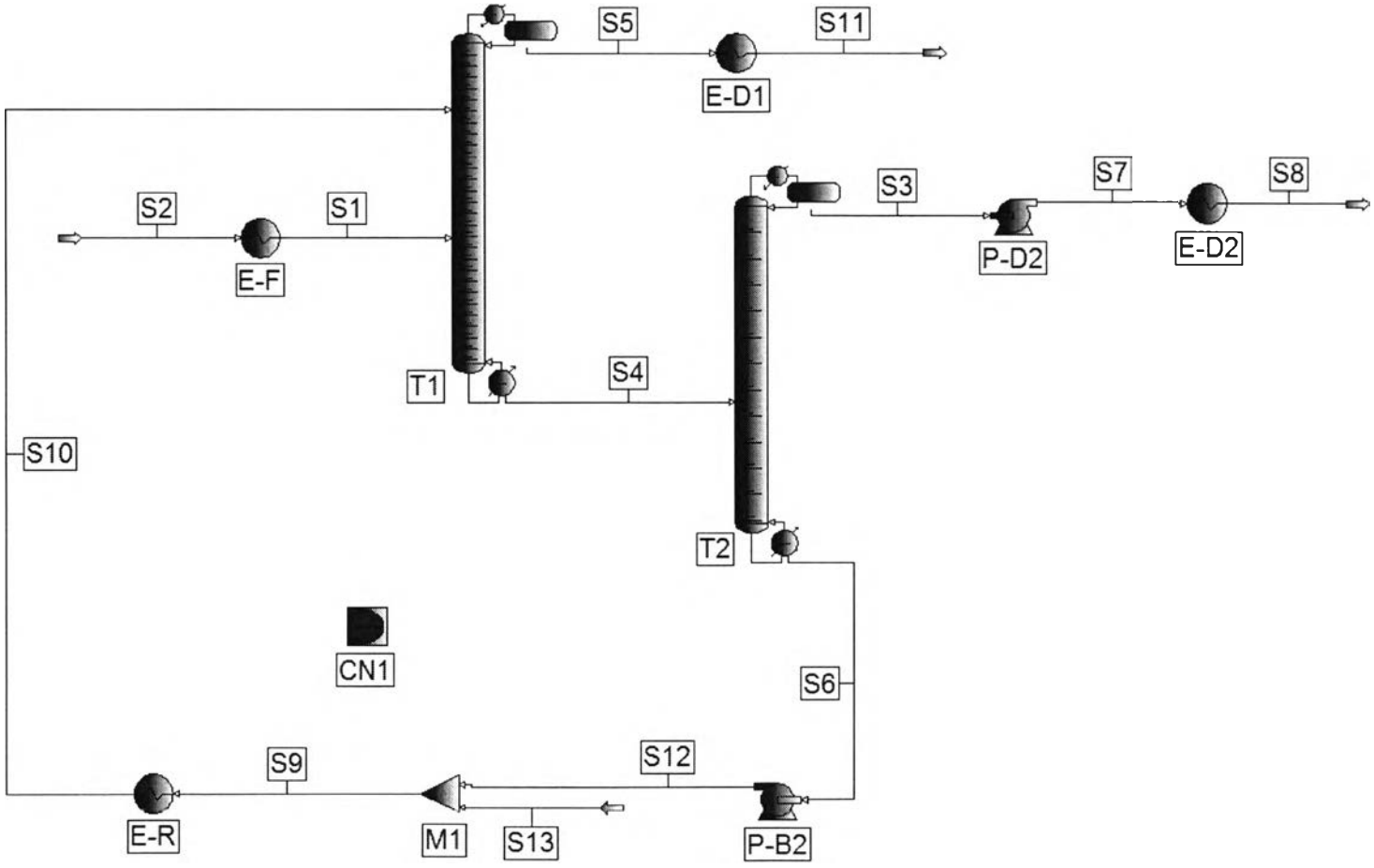

Figure G11 CS process flowsheet using NMP in toluene + MCH mixture.

Table G48 Distillation column properties of the CS process using NMP in toluene + MCH mixture

Column Name	**Unit**	**T1**	**T2**
Condenser Duty	MM WATT	-9.9503	-10.5563
Reboiler Duty	MM WATT	13.8558	11.3356
Column Total Molar Feed	KG-MOL/HR	2376.9771	2075.6169
Column Total Wt. Feed	KG/HR	230455.6767	200866.6484
Column Condenser Pres	KPA	100.0000	40.0000
Column Condenser Temp	C	100.3710	80.8510
Column Reflux Rate	KG-MOL/HR	844.8503	384.7297
Column Reflux Ratio		2.8035	0.5496

Table G49 Pump properties of the CS process using NMP in toluene + MCH mixture

Pump Name	**Unit**	**P-D2**	**P-B2**
Pump Description			
Pressure Gain	KPA	60.0000	60.0000
Head	M	7.5468	6.7810
Work	KW	1.3253	2.5171

Table G50 Heat exchanger properties of the separation process using NMP in toluene + MCH mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**
Hx Description					
Duty	MM WATT	5.3841	3.8269	1.2044	1.6742
MTD	C	97.3198	83.3746	20.9476	15.6658

Table G51 Stream table of the CS process using NMP in toluene + MCH mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S2	S3
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	101	101	30	167.7918555	25	25	80.85098732
Pressure	KPA	100	100	100	100	100	100	40
Total Mass Rate	KG/HR	93954.81186	136500.8649	29589.02828	136358.8144	535.8288126	93954.81186	64507.83407
Flowrate	KG-MOL/HR	1000	1376.977138	301.3602047	1375.544214	5.405173071	1000	700.0727199
Total Weight Comp. Rates	KG/HR							
MCH		29456.44913	1.96224558e-006	29426.99286	1.962231369e-006	0	29456.44913	29.45626417
TOLUENE		64498.36273	32.24530113	33.53476222	32.25849032	0	64498.36273	64464.8152
NMP		0						
Total Weight Comp. Fractions								
MCH		0.3135171956	1.437533441e-011	0.9945238005	1.439020557e-011	0	0.3135171956	0.0004566308045
TOLUENE		0.6864828044	0.0002362278155	0.001133351251	0.0002365706278	0	0.6864828044	0.9993331218
NMP		0	0.9997637722	0.004342848234	0.9997634294	1	0	0.0002102474357
Total Molar Comp. Rates	KG-MOL/HR							
MCH		300	1.998454299e-008	299.7000019	1.998439826e-008	0	300	0.2999981163
TOLUENE		700	0.3499578878	0.3639523944	0.35010103	0	700	699.635909
NMP		0	1376.62718	1.296250382	1375.194113	5.405173071	0	0.1368127931
Composition								
MCH		0.3	1.451334407e-011	0.9944909688	1.452835762e-011	0	0.3	0.00042852422
TOLUENE		0.7	0.0002541493813	0.001207698922	0.0002545181947	0	0.7	0.9993760492
NMP		0	0.9997458506	0.004301332298	0.9997454818	1	0	0.0001954265453

Table G51 Stream table of the CS process using NMP in toluene + MCH mixture (Continued)

Stream Name	Unit	S4	S5	S6	S7	S8	S9
Stream Description							
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	131.8472045	100.3709893	167.7784043	80.86803723	30	167.2964471
Pressure	KPA	100	100	40	100	100	100
Total Mass Rate	KG/HR	200866.6485	29589.02828	136358.8144	64507.83407	64507.83407	136500.8649
Flowrate	KG-MOL/HR	2075.616934	301.3602047	1375.544214	700.0727199	700.0727199	1376.977138
Total Weight Comp. Rates	KG/HR						
MCH		29.45626566	29426.99286	1.962231369e-006	29.45626417	29.45626417	1.96224558e-006
TOLUENE		64497.07327	33.53476222	32.25849032	64464.8152	64464.8152	32.24530113
NMP		136340.1189					
Total Weight Comp. Fractions							
MCH		0.0001466458762	0.9945238005	1.439020557e-011	0.0004566308045	0.0004566308045	1.437533441e-011
TOLUENE		0.3210939883	0.001133351251	0.0002365706278	0.9993331218	0.9993331218	0.0002362278155
NMP		0.6787593658	0.004342848234	0.9997634294	0.0002102474357	0.0002102474357	0.9997637722
Total Molar Comp. Rates	KG-MOL/HR						
MCH		0.2999981315	299.7000019	1.998439826e-008	0.2999981163	0.2999981163	1.998454299e-008
TOLUENE		699.9860055	0.3639523944	0.35010103	699.635909	699.635909	0.3499578878
NMP		1375.33093	1.296250382	1375.194113	0.1368127931	0.1368127931	1376.62718
Composition							
MCH		0.0001445344402	0.9944909688	1.452835762e-011	0.00042852422	0.00042852422	1.451334407e-011
TOLUENE		0.3372423852	0.001207698922	0.0002545181947	0.9993760492	0.9993760492	0.0002541493813
NMP		0.6626130804	0.004301332298	0.9997454818	0.0001954265453	0.0001954265453	0.9997458506

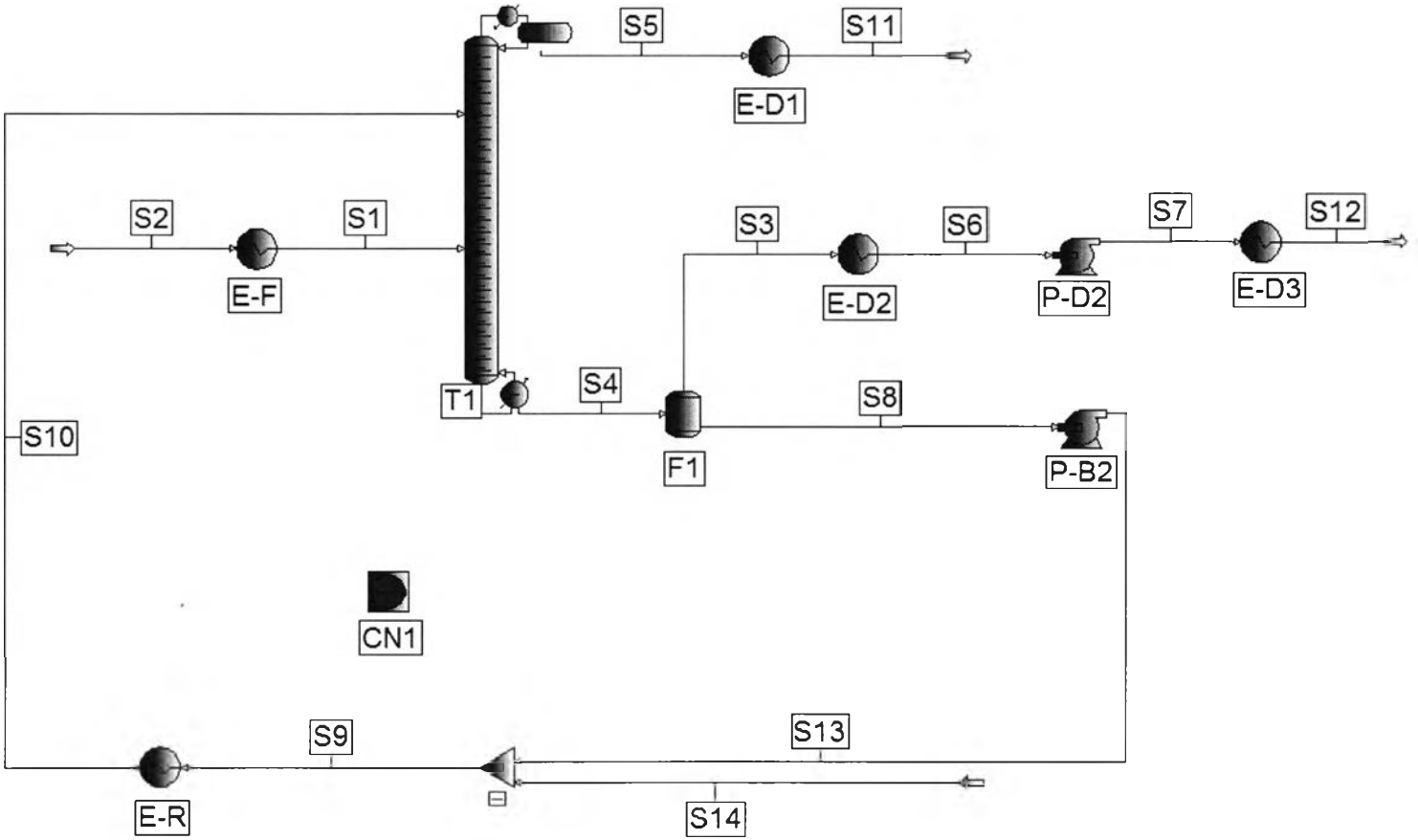

Figure G12 CS process flowsheet using [HMIM][TCB] in toluene + MCH mixture.

Table G52 Distillation column properties of the CS process using [HMIM][TCB] in toluene + MCH mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-7.9386
Reboiler Duty	MM WATT	11.3431
Column Total Molar Feed	KG-MOL/HR	1251.2843
Column Total Wt. Feed	KG/HR	164840.9091
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	100.3295
Column Reflux Rate	KG-MOL/HR	615.6936
Column Reflux Ratio		2.0478

Table G53 Flash properties of the separation process using [HMIM][TCB] in toluene + MCH mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	149.2246
Pressure	KPA	0.1000
DP	KPA	99.9000
Duty	MM WATT	4.9382

Table G54 Pump properties of the separation process using [HMIM][TCB] in toluene + MCH mixture

Pump Name	**Unit**	**P-B2**	**P-D2**
Pump Description			
Pressure Gain	KPA	99.9000	99.9000
Head	M	11.2526	11.1620
Work	KW	2.1714	1.9581

Table G55 Heat exchanger properties of the separation process using [HMIM][TCB] in toluene + MCH mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	0.4308	3.8269	1.2006	12.0478	1.7240
MTD	C	89.2893	47.7932	20.9369	208.4409	118.0083

Table G56 Stream table of IL process using [HMIM][TCB] in toluene + MCH mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	101	101	30	30	149.0238758	25	25
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	93954.81186	70886.09723	29512.00789	64442.80138	70886.0992	28.21589966	93954.81186
Flowrate	KG-MOL/HR	1000	251.2842708	300.662133	699.3378375	251.2843003	0.1	1000
Total Weight Comp. Rates	KG/HR							
MCH		29456.44913	0.001452493391	29367.95591	88.49321835	0.001454694298	0	29456.44913
TOLUENE		64498.36273	7.767049855	144.051983	64354.30796	7.770136025	0	64498.36273
[HMIM][TCB]		0	70878.32873	0	0.0001972582204	70878.32761	28.21589966	0
Total Weight Comp. Fractions								
MCH		0.3135171956	2.049052561e-008	0.9951188688	0.001373205641	2.052157354e-008	0	0.3135171956
TOLUENE		0.6864828044	0.000109570849	0.004881131	0.9986267913	0.000109614383	0	0.6864828044
[HMIM][TCB]		0	0.9998904087	0	3.060981463e-009	0.9998903651	1	0
Total Molar Comp. Rates	KG-MOL/HR							
MCH		300	1.479295808e-005	299.0987384	0.9012615673	1.481537328e-005	0	300
TOLUENE		700	0.08429570408	1.563394539	698.4365752	0.08432919825	0	700
[HMIM][TCB]		0	251.1999603	0	6.99103069e-007	251.1999563	0.1	0
Composition								
MCH		0.3	5.886941526e-008	0.9948001615	0.001288735599	5.895861087e-008	0	0.3
TOLUENE		0.7	0.0003354595328	0.0051998385	0.9987112634	0.0003355927853	0	0.7
[HMIM][TCB]		0	0.9996644816	0	9.996642988e-010	0.9996643483	1	0

Table G56 Stream table of IL process using [HMIM][TCB] in toluene + MCH mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	149.2245785	110.7466201	100.3295119	-30.20079473	-30.1818481	149.2245785	149.0441351
Pressure	KPA	0.1	100	100	0.1	100	0.1	100
Total Mass Rate	KG/HR	64442.80138	135328.9012	29512.00789	64442.80138	64442.80138	70886.0992	70886.09723
Flowrate	KG-MOL/HR	699.3378375	950.6221378	300.662133	699.3378375	699.3378375	251.2843003	251.2842708
Total Weight Comp. Rates	KG/HR							
MCH		88.49321835	88.49467263	29367.95591	88.49321835	88.49321835	0.001454694298	0.001452493391
TOLUENE		64354.30796	64362.0778	144.051983	64354.30796	64354.30796	7.770136025	7.767049855
[HMIM][TCB]		0.0001972582204	70878.32873	0	0.0001972582204	0.0001972582204	70878.32761	70878.32873
Total Weight Comp. Fractions								
MCH		0.001373205641	0.0006539229377	0.9951188688	0.001373205641	0.001373205641	2.052157354e-008	2.049052e-008
TOLUENE		0.9986267913	0.4755974314	0.004881131217	0.9986267913	0.9986267913	0.000109614383	0.000109570849
[HMIM][TCB]		3.060981463e-009	0.5237486457	0	3.060981463e-009	3.060981463e-009	0.9998903651	0.9998904087
Total Molar Comp. Rates	KG-MOL/HR							
MCH		0.9012615673	0.9012763784	299.0987384	0.9012615673	0.9012615673	1.481537328e-005	1.479295e-005
TOLUENE		698.4365752	698.5209012	1.563394539	698.4365752	698.4365752	0.08432919825	0.08429570408
[HMIM][TCB]		6.99103069e-007	251.1999603	0	6.99103069e-007	6.99103069e-007	251.1999563	251.1999603
Composition								
MCH		0.001288735599	0.0009480910896	0.9948001615	0.001288735599	0.001288735599	5.895861087e-008	5.886941e-008
TOLUENE		0.9987112634	0.7348039493	0.005199838517	0.9987112634	0.9987112634	0.0003355927853	0.0003354595328
[HMIM][TCB]		9.996642988e-010	0.2642479596	0	9.996642988e-010	9.996642988e-010	0.9996643483	0.9996644816

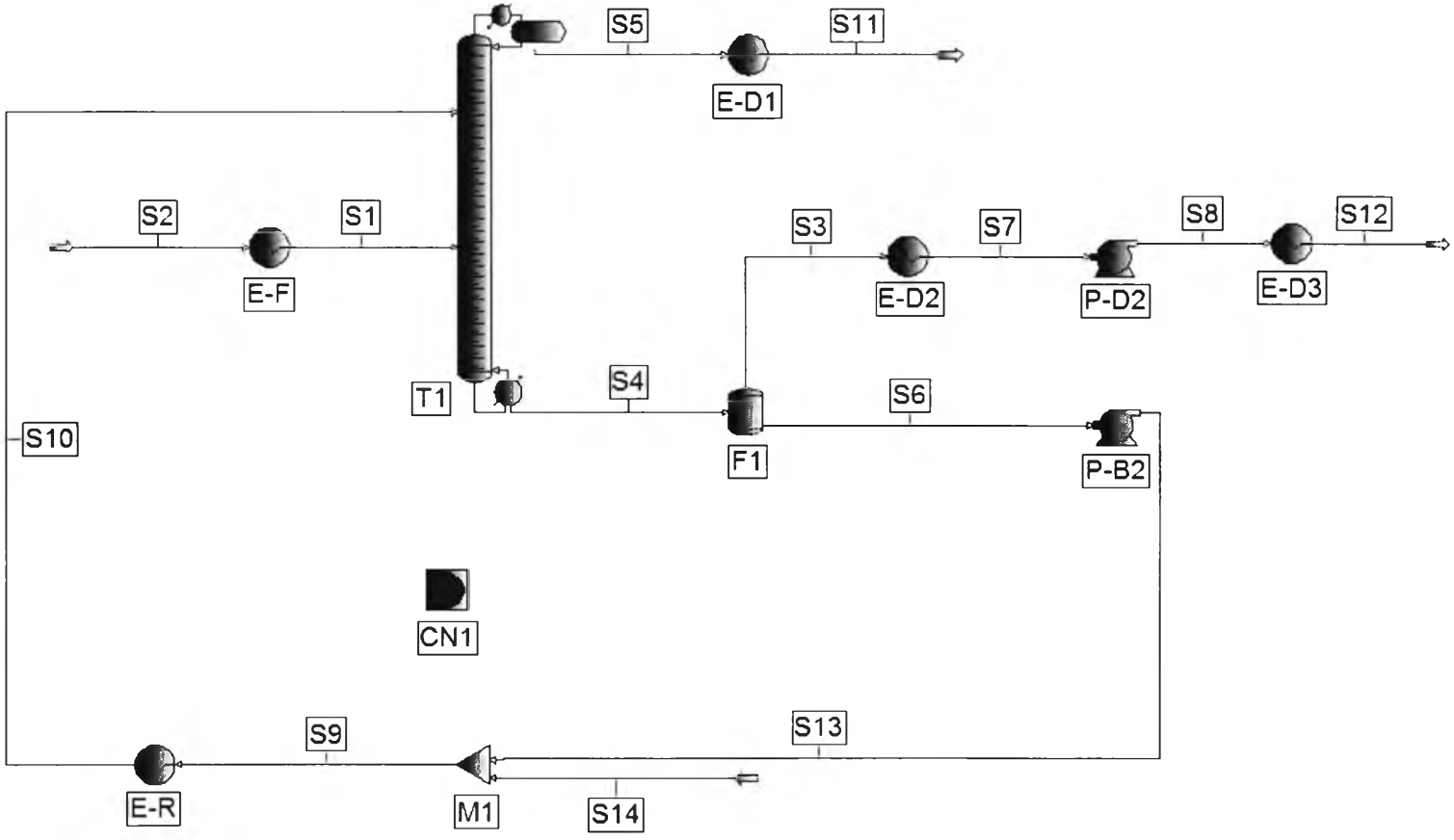

Figure G13 IL process flowsheet using [HMIM][BTI] in toluene + MCH mixture.

Table G57 Distillation column properties of the IL process using [HMIM][BTI] in toluene + MCH mixture

Column Name	**Unit**	**T1**
Column Description		
Condenser Duty	MM WATT	-13.4720
Reboiler Duty	MM WATT	12.0736
Column Total Molar Feed	KG-MOL/HR	1500.0135
Column Total Wt. Feed	KG/HR	317656.0561
Column Condenser Pres	KPA	100.0000
Column Condenser Temp	C	100.3297
Column Reflux Rate	KG-MOL/HR	1254.4000
Column Reflux Ratio		4.1717

Table G58 Flash properties of the IL process using [HMIM][BTI] in toluene + MCH mixture

Flash Name	**Unit**	**F1**
Flash Description		
Temperature	C	210.2599
Pressure	KPA	0.1000
DP	KPA	99.9000
Duty	MM WATT	11.9871

Table G59 Pump properties of the IL process using [HMIM][BTI] in toluene + MCH mixture

Pump Name	**Unit**	**P-D2**	**P-B2**
Pump Description			
Pressure Gain	KPA	99.9000	99.9000
Head	M	11.1620	8.4525
Work	KW	1.9580	5.1472

Table G60 Heat exchanger properties of the IL process using [HMIM][BTI] in toluene + MCH mixture

Hx Name	**Unit**	**E-R**	**E-F**	**E-D1**	**E-D2**	**E-D3**
Hx Description						
Duty	MM WATT	0.8102	3.8269	1.2007	13.9151	1.7240
MTD	C	114.9605	47.7932	20.9369	231.1983	118.0082

Table G61 Stream table of the IL process using [HMIM][BTI] in toluene + MCH mixture

Stream Name	Unit	S1	S10	S11	S12	S13	S14	S2
Stream Description								
Phase		Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	101	101	30	30	210.3905214	25	25
Pressure	KPA	100	100	100	100	100	100	100
Total Mass Rate	KG/HR	93954.81186	223701.2442	29514.82454	64439.98747	223701.2447	n/a	93954.81186
Flowrate	KG-MOL/HR	1000	500.0135289	300.6923561	699.3076429	500.01353	-0.02028787862	1000
Total Weight Comp. Rates	KG/HR							
MCH		29456.44913	0.0003737264317	29368.4734	87.97572716	0.0003717913243	0	29456.44913
TOLUENE		64498.36273	1.246033084	146.3511375	64352.01143	1.246041453	0	64498.36273
[HMIM][BTI]		0	223699.9978	0	0.0003128617693	223699.9983	-9.07679677	0
Total Weight Comp. Fractions								
MCH		0.3135171956	1.670649768e-009	0.9950414363	0.001365235013	1.661999355e-009	0	0.3135171956
TOLUENE		0.6864828044	5.570076683e-006	0.004958563	0.9986347601	5.570114083e-006	0	0.6864828044
[HMIM][BTI]		0	0.9999944283	0	4.85508737e-009	0.9999944282	1	0
Total Molar Comp. Rates	KG-MOL/HR							
MCH		300	3.806226916e-006	299.1040089	0.8959911642	3.786518762e-006	0	300
TOLUENE		700	0.01352318295	1.588347237	698.411651	0.01352327377	0	700
[HMIM][BTI]		0	500.0000019	0	6.992887206e-007	500.0000029	-0.02028787862	0
Composition								
MCH		0.3	7.61224786e-009	0.9947177	0.001281254643	7.572832604e-009	0	0.3
TOLUENE		0.7	2.70456341e-005	0.00528230	0.9987187444	2.704581569e-005	0	0.7
[HMIM][BTI]		0	0.9999729468	0	9.999729414e-010	0.9999729466	1	0

Table G61 Stream table of the IL process using [HMIM][BTI] in toluene + MCH mixture (Continued)

Stream Name	Unit	S3	S4	S5	S6	S7	S8	S9
Stream Description								
Phase		Vapor	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid
Temperature	C	210.2598866	109.0664987	100.3297456	210.2598866	-30.20063363	-30.18168702	210.3906364
Pressure	KPA	0.1	100	100	0.1	0.1	100	100
Total Mass Rate	KG/HR	64439.98747	288141.2315	29514.82454	223701.2447	64439.98747	64439.98747	223701.2442
Flowrate	KG-MOL/HR	699.3076429	1199.321173	300.6923561	500.01353	699.3076429	699.3076429	500.0135289
Total Weight Comp. Rates	KG/HR							
MCH		87.97572716	87.97609916	29368.4734	0.0003717913243	87.97572716	87.97572716	0.0003737264317
TOLUENE		64352.01143	64353.25763	146.3511375	1.246041453	64352.01143	64352.01143	1.246033084
[HMIM][BTI]		0.0003128617693	223699.9978	0	223699.9983	0.0003128617693	0.0003128617693	223699.9978
Total Weight Comp. Fractions								
MCH		0.001365235013	0.0003053228401	0.9950414363	1.661999355e-009	0.001365235013	0.001365235013	1.670649e-009
TOLUENE		0.9986347601	0.2233392885	0.004958563698	5.570114083e-006	0.9986347601	0.9986347601	5.570076e-006
[HMIM][BTI]		4.85508737e-009	0.7763553887	0	0.9999944282	4.85508737e-009	4.85508737e-009	0.9999944283
Total Molar Comp. Rates	KG-MOL/HR							
MCH		0.8959911642	0.8959949529	299.1040089	3.786518762e-006	0.8959911642	0.8959911642	3.80622e-006
TOLUENE		698.411651	698.4251759	1.588347237	0.01352327377	698.411651	698.411651	0.01352318295
[HMIM][BTI]		6.992887206e-007	500.0000019	0	500.0000029	6.992887206e-007	6.992887206e-007	500.0000019
Composition								
MCH		0.001281254643	0.0007470850787	0.9947177	7.572832604e-009	0.001281254643	0.001281254643	7.61224786e-009
TOLUENE		0.9987187444	0.5823504094	0.005282300016	2.704581569e-005	0.9987187444	0.9987187444	2.70456341e-005
[HMIM][BTI]		9.999729414e-010	0.4169025056	0	0.9999729466	9.999729414e-010	9.999729414e-010	0.9999729468

Appendix H Supplementary Data in Economic Comparison Step

- **Water + Ethanol Mixture**
  - EG (Table H1-H5)
  - [MMIM][DMP] (Table H6-H10)
- **Ethanol + Hexane Mixture**
  - Sulfolane (Table H11-H15)
  - [EMIM][BTI] (Table H16-H20)
- **Benzene + Hexane Mixture**
  - NMP (Table H21-H25)
  - [EMIM][EtSO4] (Table H26-H30)
- **Toluene + MCH Mixture**
  - NMP (Table H31-H35)
  - [HMIM][TCB] (Table H36-H40)

Table H1 Sizing equipment of CS process in water + ethanol mixture using EG

Sizing equipment of CS process in water + ethanol mixture using EG				
Column				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	2	m	2	m
Pressure	100	kPa	100	kPa
Material	316 SS		316 SS	
Number	30	stages	15	stages
Height	23.69	m	14.54	m
Tray				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	1.3	m	1.1	m
Number	28	trays	13	trays
Material	316 SS		316 SS	
Type	valve tray		valve tray	
Spacing	0.61 m	m	0.61 m	m
Condenser				
Topic	**T1**	**Unit**	**T2**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	-2.9892	MMWATT	-0.9224	MMWATT
Stream in	78	^{o}C	59.1	^{o}C
Stream out	77.971	^{o}C	58.931	^{o}C
utility	CW		CW	
in	25	^{o}C	25	^{o}C
out	45	^{o}C	45	^{o}C
LMTD	42.20083938	^{o}C	22.58259289	^{o}C
UA	0.070832714	kW/C	0.04084562	kW/C

Table H1 Sizing equipment of CS process in water + ethanol mixture using EG (Continued)

Condenser				
Topic	**T1**	**Unit**	**T2**	**Unit**
U	500	W/m^2C	1250	W/m^2C
A	0.141665429	m^2	0.032676496	m^2
Type U	Water to organic vapors		Water to aqueous vapors	
Reboiler				
Topic	**T1**	**Unit**	**T2**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	3.9095	MMWATT	0.7842	MMWATT
Stream in	155.072	°C	150.682	°C
Stream out	155.1	°C	150.8	°C
utility	LPS		LPS	
in	160	°C	160	°C
out	160	°C	160	°C
LMTD	-4.913986705	°C	-9.258874679	°C
UA	795.5861981	kW/C	84.69711787	kW/C
U	750	W/m^2C	1250	W/m^2C
A	1060.781598	m^2	67.75769429	m^2
Type U	Steam to light organic		Steam to light organic	

Table H1 Sizing equipment of CS process in water + ethanol mixture using EG (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa
Flowrate	723.558	kg/hr	13032.858	kg/hr
Capacity	0.000202	m3/s	0.003268	m3/s
Mixer				
Topic	**M-1**	**Unit**		**Unit**
Material	316 SS			
Capacity	0.003268	m3/s		
Heat exchanger				
Topic	**EF**	**Unit**	**ED1**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	0.4355	MMWATT	0.3432	MMWATT
Stream in	25	°C	77.971	°C
Stream out	78	°C	30	°C
utility	LPS		CW	
LMTD	65.4246	°C	14.8293	°C
UA	6.656517579	kW/C	23.14337157	kW/C
U	750	W/m^2C	500	W/m^2C
A	8.875356772	m^2	46.28674314	m^2

Table H1 Sizing equipment of CS process in water + ethanol mixture using EG (Continued)

Heat exchanger				
Topic	**EF**	**Unit**	**ED1**	**Unit**
Type U	Steam to organic solvents		Water to organic solvents	
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	0.8219	MMWATT	0.0301	MMWATT
Stream in	150.637	°C	58.935	°C
Stream out	78	°C	30	°C
utility	CW		CW	
LMTD	76.3167	°C	8.7175	°C
UA	10.76959565	kW/C	3.452824778	kW/C
U	500	W/m^2C	1500	W/m^2C
A	21.53919129	m^2	2.301883185	m^2
Type U	Water to organic solvents		Water to aqueous solution	

Table H2 Purchase equipment cost calculation of CS process in water + ethanol mixture using EG

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST
T-1	Tower Unit	23.69	meters	316 Stainless Steel	$ 403,695.00
tT-1	Valve tray	28	trays	Stainless Steel	$ 58,900.00
rT-1	Heat Exchanger	1060.782	sq.meter	316 Stainless Steel	$ 174,562.00
cT-1	Heat Exchanger	0.142	sq.meter	316 Stainless Steel	$ 6,039.00
T-2	Tower Unit	14.54	meters	316 Stainless Steel	$ 259,256.00
tT-2	Valve tray	13	trays	Stainless Steel	$ 31,781.00
rT-2	Heat Exchanger	67.758	sq.meter	316 Stainless Steel	$ 23,182.00
cT-2	Heat Exchanger	0.0327	sq.meter	316 Stainless Steel	$ 6,039.00
P-1	Pump	0.000202	cubic meter/s	Stainless Steel	$ 4,194.00
P-2	Pump	0.003268	cubic meter/s	Stainless Steel	$ 7,161.00
M-1	Mixer	0.003268	cubic meters	Stainless Steel	$ 8,970.00
E-1	Heat Exchanger	8.875	sq.meter	316 Stainless Steel	$ 7,468.00
E-2	Heat Exchanger	46.287	sq.meter	316 Stainless Steel	$ 17,452.00
E-3	Heat Exchanger	21.539	sq.meter	316 Stainless Steel	$ 10,848.00
E-4	Heat Exchanger	2.302	sq.meter	316 Stainless Steel	$ 6,039.00
				Total	$ 1,025,586.00

Table H3 Utility cost calculation of CS process in water + ethanol mixture using EG

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST	
T-1	Tower Unit	n/a	n/a	n/a	n/a	$	-
tT-1	Valve tray	n/a	n/a	n/a	n/a	$	-
rT-1	Heat Exchanger	LP steam	3909.5	kW	0.01	$	1,489.00
cT-1	Heat Exchanger	Cooling water	2989.2	kW	3.769999981	$	291,945.00
T-2	Tower Unit	n/a	n/a	n/a	n/a	$	-
tT-2	Valve tray	n/a	n/a	n/a	n/a	$	-
rT-2	Heat Exchanger	LP steam	784.2	kW	0.01	$	299.00
cT-2	Heat Exchanger	Cooling water	922.4	kW	3.769999981	$	90,088.00
P-1	Pump	n/a	n/a	n/a	n/a	$	-
P-2	Pump	n/a	n/a	n/a	n/a	$	-
M-1	Mixer	Electricity	0	kW	23.25	$	-
E-1	Heat Exchanger	LP steam	435.5	kW	0.01	$	166.00
E-2	Heat Exchanger	Cooling water	343.2	kW	3.769999981	$	33,519.00
E-3	Heat Exchanger	Cooling water	821.9	kW	3.769999981	$	80,272.00
E-4	Heat Exchanger	Cooling water	30.1	kW	3.769999981	$	2,940.00
					Total	$	500,718.00

Table H4 CAPEX calculation of CS process in water + ethanol mixture using EG

Purchase Equipment Cost	**$ 1,025,586.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 1,128,144.60
Purchased Equipment Installation	0.47	$ 530,227.96
Instrumentation and Controls (installed)	0.36	$ 406,132.06
Piping (Installed)	0.68	$ 767,138.33
Electrical Systems (Installed)	0.11	$ 124,095.91
Buildings (Including Services)	0.18	$ 203,066.03
Yard Improvement	0.1	$ 112,814.46
Service Facilities (Installed)	0.7	$ 789,701.22
	Total Direct Cost	$ 4,061,320.56

Table H4 CAPEX calculation of CS process in water + ethanol mixture using EG (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Engineering and Supervision	0.33	$ 372,287.72
Construction Expenses	0.41	$ 462,539.29
Legal Expenses	0.04	$ 45,125.78
Contractor's Fees	0.22	$ 248,191.81
Contingency	0.44	$ 496,383.62
	Total indirect cost	$ 1,624,528.22
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Fixed-capital Investment (FCI)		$ 5,685,848.78
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Working Capital Investment (WC)	0.89	$ 22,562.89
CAPEX	**Total Capital Investment (TCI)**	**$ 5,708,411.68**

Table H5 OPEX calculation of CS process in water + ethanol mixture using EG

Fixed Capital Investment		**$ 5,685,848.78**	
Plant Capacity		**507019.3896**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 852,877.38
Operating Supervision	0.15	Operating Labor	$ 127,931.61
Utilities	0		$ 500,718.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 341,150.94
Operating Supplies	0.15	Maintenance and Supplies	$ 51,172.64
Laboratory Charges	0.15	Operating Labor	$ 127,931.61
Royalties	0.01	Total Product Cost	$ 24,059.51
		Variable Cost	$ 2,025,841.68
Property Taxes	0.02	Fixed Capital Investment	$ 113,716.98
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 56,858.49
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 170,575.47

Table H5 OPEX calculation of CS process in water + ethanol mixture using EG (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenace	$ 793,175.93
		Manufacturing Cost	$ 2,196,417.15
Administration	0.2	Labor + Supervision + Maintenace	$ 264,391.98
Distribution & selling	0.04	Total Product Cost	$ 96,238.03
Research & Development	0.04	Total Product Cost	$ 96,238.03
		General Expense	$ **456,868.04**
OPEX	**Total Product Cost with Out Depreciation**		$ **2,405,950.75**

Table H6 Sizing equipment of IL process in water + ethanol mixture using [MMIM][DMP]

Sizing equipment of IL process in water + ethanol mixture using [MMIM][DMP]				
Column				
Topic	**T1**	**Unit**		
Diameter	2	m		
Pressure	100	kPa		
Material	316 SS			
Number	30	stages		
Height	23.69	m		
Tray				
Topic	**T1**	**Unit**		
Diameter	1.3	m		
Number	28	trays		
Material	316 SS			
Type	valve tray			
Spacing	0.61 m	m		
Condenser				
Topic	**T1**	**Unit**		
Type	Shell & Tube			
Material	316 SS			
Duty	-3.1623	MMWATT		
Stream in	78	°C		
Stream out	77.97	°C		
utility	CW			
in	25	°C		
out	45	°C		
LMTD	42.20040974	°C		

Table H6 Sizing equipment of IL process in water + ethanol mixture using [MMIM][DMP] (Continued)

Condenser				
Topic	**T1**	**Unit**		
UA	0.074935291	kW/C		
U	500	W/m^2C		
A	0.149870583	m^2		
Type U	Water to organic vapors			
Reboiler				
Topic	**T1**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	3.2476	MMWATT		
Stream in	98	°C		
Stream out	109.4	°C		
utility	LPS			
in	161	°C		
out	161.027	°C		
LMTD	-57.12313737	°C		
UA	56.85261961	kW/C		
U	750	W/m^2C		
A	75.80349281	m^2		
Type U	Steam to light organic			
Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa

Table H6 Sizing equipment of IL process in water + ethanol mixture using [MMIM][DMP] (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Flowrate	722.94	kg/hr	8888.941	kg/hr
Capacity	0.000202	m3/s	0.002014	m3/s
Mixer				
Topic	**M-1**	**Unit**		**Unit**
Material	316 SS			
Capacity	0.002014	m3/s		
Heat exchanger				
Topic	**E-1**	**Unit**	**E-3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	0.4355	MMWATT	0.3433	MMWATT
Stream in	25	°C	77.97	°C
Stream out	78	°C	30	°C
utility	LPS		CW	
LMTD	65.4246	°C	14.8291	°C
UA	6.656517579	kW/C	23.1504272	kW/C
U	750	W/m^2C	500	W/m^2C
A	8.875356772	m^2	46.3008544	m^2
Type U	Steam to organic solvents		Water to organic solvents	

Table H6 Sizing equipment of IL process in water + ethanol mixture using [MMIM][DMP] (Continued)

Heat exchanger				
Topic	**E2**	**Unit**	**E-5**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	0.1445	MMWATT	0.0247	MMWATT
Stream in	222.711	°C	5.804	°C
Stream out	78	°C	30	°C
utility	CW		LPS	
LMTD	103.0784	°C	102.0843	°C
UA	1.401845585	kW/C	0.241956892	kW/C
U	500	W/m^2C	750	W/m^2C
A	2.803691171	m^2	0.32260919	m^2
Type U	Water to organic solvents		Steam to organic solvents	
Topic	**E-4**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	0.606	MMWATT		
Stream in	222.634	°C		
Stream out	5.801	°C		
utility	NG			
LMTD	261.0207	°C		

Table H6 Sizing equipment of IL process in water + ethanol mixture using [MMIM][DMP] (Continued)

Heat exchanger				
Topic	**E-4**	**Unit**		
UA	2.321654949	kW/C		
U	35	W/m^2C		
A	66.33299855	m^2		
Type U	Gases to Gases			
Flash drum				
Topic	**V-1**	**Unit**		
type	Vertical			
Pressure	101.3	kPa		
Diameter	0.75	m		
Height	3	m		

Table H7 Purchase equipment cost calculation of IL process in water + ethanol mixture using [MMIM][DMP]

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST
T-1	Tower Unit	23.69	meters	316 Stainless Steel	$ 403,695.00
tT-1	Valve tray	28	trays	Stainless Steel	$ 58,900.00
rT-1	Heat Exchanger	75.803	sq.meter	316 Stainless Steel	$ 25,329.00
cT-1	Heat Exchanger	0.1499	sq.meter	316 Stainless Steel	$ 6,039.00
P-1	Pump	0.000202	cubic meter/s	Stainless Steel	$ 4,194.00
P-2	Pump	0.002014	cubic meter/s	Stainless Steel	$ 6,124.00
M-1	Mixer	0.002014	cubic meters	Stainless Steel	$ 8,970.00
E-1	Heat Exchanger	8.875	sq.meter	316 Stainless Steel	$ 7,468.00
E-2	Heat Exchanger	2.804	sq.meter	316 Stainless Steel	$ 6,039.00
E-3	Heat Exchanger	46.3	sq.meter	316 Stainless Steel	$ 17,455.00
E-4	Heat Exchanger	66.333	sq.meter	316 Stainless Steel	$ 22,802.00
E-5	Heat Exchanger	0.3226	sq.meter	316 Stainless Steel	$ 6,039.00
V-1	Vessel	3	meters	316 Stainless Steel	$ 39,100.00
				Total	**$ 612,154.00**

Table H8 Utility cost calculation of IL process in water + ethanol mixture using [MMIM][DMP]

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST
T-1	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-1	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-1	Heat Exchanger	LP steam	3247.6	kW	0.01	$ 1,237.00
cT-1	Heat Exchanger	Cooling water	3162.3	kW	3.769999981	$ 308,851.00
P-1	Pump	n/a	n/a	n/a	n/a	$ -
P-2	Pump	n/a	n/a	n/a	n/a	$ -
M-1	Mixer	Electricity	0	kW	23.25	$ -
E-1	Heat Exchanger	LP steam	435.5	kW	0.01	$ 166.00
E-2	Heat Exchanger	Cooling water	144.5	kW	3.769999981	$ 14,113.00
E-3	Heat Exchanger	Cooling water	343.3	kW	3.769999981	$ 33,529.00
E-4	Heat Exchanger	Cooling water	606	kW	3.769999981	$ 59,186.00
E-5	Heat Exchanger	LP steam	24.7	kW	0.01	$ 9.00
V-1	Vessel	n/a	n/a	n/a	n/a	$ -
					Total	**$ 417,091.00**

Table H9 CAPEX calculation of IL process in water + ethanol mixture using [MMIM][DMP]

Purchase Equipment Cost	**$ 612,154.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 673,369.40
Purchased Equipment Installation	0.47	$ 316,483.62
Instrumentation and Controls (installed)	0.36	$ 242,412.98
Piping (Installed)	0.68	$ 457,891.19
Electrical Systems (Installed)	0.11	$ 74,070.63
Buildings (Including Services)	0.18	$ 121,206.49
Yard Improvement	0.1	$ 67,336.94
Service Facilities (Installed)	0.7	$ 471,358.58
	Total Direct Cost	$ 2,424,129.84

Table H9 CAPEX calculation of IL process in water + ethanol mixture using [MMIM][DMP] (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Engineering and Supervision	0.33	$ 222,211.90
Construction Expenses	0.41	$ 276,081.45
Legal Expenses	0.04	$ 26,934.78
Contractor's Fees	0.22	$ 148,141.27
Contingency	0.44	$ 296,282.54
	Total indirect cost	$ 969,651.94
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Fixed-capital Investment (FCI)		$ 3,393,781.78
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Working Capital Investment (WC)	0.89	$ 13,467.39
CAPEX	**Total Capital Investment (TCI)**	**$ 3,407,249.16**

Table H10 OPEX calculation of IL process in water + ethanol mixture using [MMIM][DMP]

Fixed Capital Investment		**$ 3,393,781.78**	
Plant Capacity		**407534.5152**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 509,067.28
Operating Supervision	0.15	Operating Labor	$ 76,360.09
Utilities	0		$ 417,091.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 203,626.92
Operating Supplies	0.15	Maintenance and Supplies	$ 30,544.04
Laboratory Charges	0.15	Operating Labor	$ 76,360.09
Royalties	0.01	Total Product Cost	$ 15,659.83
		Variable Cost	$ 1,328,709.25
Property Taxes	0.02	Fixed Capital Investment	$ 67,875.64
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 33,937.82
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 101,813.46

Table H10 OPEX calculation of IL process in water + ethanol mixture using [MMIM][DMP] (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenace	$ 473,432.59
		Manufacturing Cost	$ 1,430,522.71
Administration	0.2	Labor + Supervision + Maintenace	$ 157,810.86
Distribution & selling	0.04	Total Product Cost	$ 62,639.31
Research & Development	0.04	Total Product Cost	$ 62,639.31
		General Expense	$ 283,089.48
OPEX	**Total Product Cost with Out Depreciation**		**$ 1,565,982.75**

Table H11 Sizing equipment of CS process in ethanol + hexane mixture using sulfolane

Sizing equipment of CS process in ethanol + hexane mixture using sulfolane				
Column				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	2	m	3	m
Pressure	100	kPa	100	kPa
Material	316 SS		316 SS	
Number	7	stages	5	stages
Height	9.66	m	8.44	m
Tray				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	2	m	3	m
Number	5	trays	3	trays
Material	316 SS		316 SS	
Type	valve tray		valve tray	
Spacing	0.61 m	m	0.61 m	m
Condenser				
Topic	**T1**	**Unit**	**T2**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	-5.7822	MMWATT	-7.763	MMWATT
Stream in	67.6	°C	84.8	°C
Stream out	67.557	°C	77.8	°C
utility	CW		CW	
in	25	°C	25	°C
out	45	°C	45	°C

Table H11 Sizing equipment of CS process in ethanol + hexane mixture using sulfolane (Continued)

Condenser				
Topic	**T1**	**Unit**	**T2**	**Unit**
LMTD	31.53290423	°C	45.99420895	°C
UA	0.18337036	kW/C	0.168782118	kW/C
U	500	W/m^2C	500	W/m^2C
A	0.36674072	m^2	0.337564236	m^2
Type U	Water to organic vapors		Water to organic vapors	
Reboiler				
Topic	**T1**	**Unit**	**T2**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	6.4114	MMWATT	29.0894	MMWATT
Stream in	80.1	°C	186.1	°C
Stream out	88.7	°C	284.9	°C
utility	LPS		LPS	
in	160	°C	160	°C
out	160	°C	160	°C
LMTD	-75.51840397	°C	63.10767877	°C
UA	84.89851033	kW/C	460.9486606	kW/C
U	750	W/m^2C	750	W/m^2C
A	113.1980138	m^2	614.5982141	m^2
Type U	Steam to light organic		Steam to light organic	

Table H11 Sizing equipment of CS process in ethanol + hexane mixture using sulfolane (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type				
Material				
Pressure		kPa		kPa
Flowrate		kg/hr		kg/hr
Capacity		m3/s		m3/s
Mixer				
Topic	M-1	**Unit**		**Unit**
Material	316 SS			
Capacity	0.03939	m3/s		
Heat exchanger				
Topic	**E2**	**Unit**	**E3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	1.638	MMWATT	0.6483	MMWATT
Stream in	25	^{o}C	67.557	^{o}C
Stream out	59	^{o}C	30	^{o}C
utility	LPS		CW	
LMTD	77.2204	^{o}C	11.6533	^{o}C
UA	21.21201133	kW/C	55.63231016	kW/C
U	750	W/m^2C	500	W/m^2C
A	28.28268178	m^2	111.2646203	m^2
Type U	Steam to organic solvents		Water to organic solvents	

Table H11 Sizing equipment of CS process in ethanol + hexane mixture using sulfolane (Continued)

Heat exchanger				
Topic	**E1**	**Unit**	**E4**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	21.253	MMWATT	1.4958	MMWATT
Stream in	284.837	°C	77.755	°C
Stream out	59	°C	30	°C
utility	CW		CW	
LMTD	105.363	°C	14.7663	°C
UA	201.712176	kW/C	101.2982264	kW/C
U	500	W/m^2C	500	W/m^2C
A	403.424352	m^2	202.5964527	m^2
Type U	Water to organic solvents		Water to organic solvents	

Table H12 Purchase equipment cost calculation of CS process in ethanol + hexane mixture using sulfolane

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST
T-1	Tower Unit	9.66	meters	316 Stainless Steel	$ 183,222.00
tT-1	Valve tray	5	trays	Stainless Steel	$ 39,977.00
rT-1	Heat Exchanger	113.22097	sq.meter	316 Stainless Steel	$ 35,315.00
cT-1	Heat Exchanger	0.36679	sq.meter	316 Stainless Steel	$ 6,039.00
T-2	Tower Unit	8.44	meters	316 Stainless Steel	$ 254,524.00
tT-2	Valve tray	3	trays	Stainless Steel	$ 54,345.00
rT-2	Heat Exchanger	873.22144	sq.meter	316 Stainless Steel	$ 174,562.00
cT-2	Heat Exchanger	0.397266	sq.meter	316 Stainless Steel	$ 6,039.00
P-1	Pump	0.011296	cubic meter/s	Stainless Steel	$ 12,742.00
P-2	Pump	0.039384	cubic meter/s	Stainless Steel	$ 20,606.00
M-1	Mixer	0.039384	cubic meters	Stainless Steel	$ 8,970.00
E-1	Heat Exchanger	390.8374	sq.meter	316 Stainless Steel	$ 109,402.00
E-2	Heat Exchanger	28.2827	sq.meter	316 Stainless Steel	$ 12,647.00
E-3	Heat Exchanger	111.2646	sq.meter	316 Stainless Steel	$ 34,793.00
E-4	Heat Exchanger	201.3184	sq.meter	316 Stainless Steel	$ 58,825.00
				Total	**$ 1,012,008.00**

Table H13 Utility cost calculation of CS process in ethanol + hexane mixture using sulfolane

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST
T-1	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-1	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-1	Heat Exchanger	LP steam	6412.7	kW	0.01	$ 2,442.00
cT-1	Heat Exchanger	Cooling water	5783	kW	3.769999981	$ 564,806.00
T-2	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-2	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-2	Heat Exchanger	LP steam	27566.1	kW	0.01	$ 10,496.00
cT-2	Heat Exchanger	Cooling water	7882.2	kW	3.769999981	$ 769,827.00
P-1	Pump	n/a	n/a	n/a	n/a	$ -
P-2	Pump	n/a	n/a	n/a	n/a	$ -
M-1	Mixer	Electricity	0	kW	23.25	$ -
E-1	Heat Exchanger	Cooling water	19837.4	kW	3.769999981	$ 1,937,451.00
E-2	Heat Exchanger	LP steam	1638	kW	0.01	$ 624.00
E-3	Heat Exchanger	Cooling water	648.3	kW	3.769999981	$ 63,317.00
E-4	Heat Exchanger	Cooling water	1270.5	kW	3.769999981	$ 124,085.00
					Total	**$ 3,473,048.00**

Table H14 CAPEX calculation of CS process in ethanol + hexane mixture using sulfolane

Purchase Equipment Cost	**$ 1,012,008.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 1,113,208.80
Purchased Equipment Installation	0.47	$ 523,208.14
Instrumentation and Controls (installed)	0.36	$ 400,755.17
Piping (Installed)	0.68	$ 756,981.98
Electrical Systems (Installed)	0.11	$ 122,452.97
Buildings (Including Services)	0.18	$ 200,377.58
Yard Improvement	0.1	$ 111,320.88
Service Facilities (Installed)	0.7	$ 779,246.16
	Total Direct Cost	$ 4,007,551.68

Table H14 CAPEX calculation of CS process in ethanol + hexane mixture using sulfolane (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Engineering and Supervision	0.33	$	367,358.90
Construction Expenses	0.41	$	456,415.61
Legal Expenses	0.04	$	44,528.35
Contractor's Fees	0.22	$	244,905.94
Contingency	0.44	$	489,811.87
	Total indirect cost	$	1,603,020.67
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Fixed-capital Investment (FCI)		$	5,610,572.35
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Working Capital Investment (WC)	0.89	$	22,264.18
CAPEX	**Total Capital Investment (TCI)**	**$**	**5,632,836.53**

Table H15 OPEX calculation of CS process in ethanol + hexane mixture using sulfolane

Fixed Capital Investment		**$ 5,610,572.35**	
Plant Capacity		**5719986.194**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 841,585.88
Operating Supervision	0.15	Operating Labor	$ 126,237.88
Utilities	0		$ 3,473,048.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 336,634.32
Operating Supplies	0.15	Maintenance and Supplies	$ 50,495.15
Laboratory Charges	0.15	Operating Labor	$ 126,237.88
Royalties	0.01	Total Product Cost	$ 56,476.79
		Variable Cost	$ 5,010,715.89
Property Taxes	0.02	Fixed Capital Investment	$ 112,211.44
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 56,105.72
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 168,317.16

Table H15 OPEX calculation of CS process in ethanol + hexane mixture using sulfolane (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenace	$ 782,674.88
		Manufacturing Cost	$ 5,179,033.05
Administration	0.2	Labor + Supervision + Maintenace	$ 260,891.63
Distribution & selling	0.04	Total Product Cost	$ 225,907.16
Research & Development	0.04	Total Product Cost	$ 225,907.16
		General Expense	$ 712,705.95
OPEX	**Total Product Cost with Out Depreciation**		**$ 5,647,679.00**

Table H16 Sizing equipment of IL process in ethanol + hexane mixture using [EMIM][BTI]

Sizing equipment of IL process in ethanol + hexane mixture using [EMIM][BTI]				
Column				
Topic	**T1**	**Unit**		
Diameter	3	m		
Pressure	100	kPa		
Material	316 SS			
Number	7	stages		
Height	9.66	m		
Tray				
Topic	**T1**	**Unit**		
Diameter	2.7	m		
Number	5	trays		
Material	316 SS			
Type	valve tray			
Spacing	0.61 m	m		
Condenser				
Topic	**T1**	**Unit**		
Type	Shell & Tube			
Material	316 SS			
Duty	-13.5843	MMWATT		
Stream in	68.3	^{o}C		
Stream out	68.268	^{o}C		
utility	CW			
in	25	^{o}C		
out	45	^{o}C		

Table H16 Sizing equipment of IL process in ethanol + hexane mixture using [EMIM][BTI] (Continued)

Condenser				
Topic	**T1**	**Unit**		
LMTD	32.26056761	°C		
UA	0.421080626	kW/C		
U	500	W/m^2C		
A	0.842161252	m^2		
Type U	Water to organic vapors			
Reboiler				
Topic	**T1**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	6.47019	MMWATT		
Stream in	98	°C		
Stream out	109.4	°C		
utility	LPS			
in	160	°C		
out	160	°C		
LMTD	-56.10710901	°C		
UA	115.3185419	kW/C		
U	750	W/m^2C		
A	153.7580558	m^2		
Type U	Steam to light organic			

Table H16 Sizing equipment of IL process in ethanol + hexane mixture using [EMIM][BTI] (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa
Flowrate	32272.6123	kg/hr	430431.6091	kg/hr
Capacity	0.01129	m3/s	0.07882	m3/s
Mixer				
Topic	M-1	**Unit**		**Unit**
Material	316 SS			
Capacity	0.07882	m3/s		
Heat exchanger				
Topic	**E-2**	**Unit**	**E-3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	1.638	MMWATT	0.6609	MMWATT
Stream in	25	°C	68.268	°C
Stream out	59	°C	30	°C
utility	LPS		CW	
LMTD	77.2204	°C	11.8805	°C
UA	21.21201133	kW/C	55.62897184	kW/C
U	750	W/m^2C	500	W/m^2C
A	28.28268178	m^2	111.2579437	m^2
Type U	Steam to organic solvents		Water to organic solvents	
Topic	**E-1**	**Unit**	**E-5**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	

Table H16 Sizing equipment of IL process in ethanol + hexane mixture using [EMIM][BTI] (Continued)

Heat exchanger				
Topic	**E-1**	**Unit**	**E-5**	**Unit**
Duty	1.9459	MMWATT	13.2858	MMWATT
Stream in	216.383	°C	-33.707	°C
Stream out	59	°C	30	°C
utility	CW		LPS	
LMTD	84.9332	°C	119.5007	°C
UA	22.91094649	kW/C	111.1775914	kW/C
U	500	W/m^2C	750	W/m^2C
A	45.82189297	m^2	148.2367886	m^2
Type U	Water to organic solvents		Steam to organic solvents	
Topic	**E-4**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	13.2858	MMWATT		
Stream in	216.172	°C		
Stream out	-33.719	°C		
utility	NG			
LMTD	230.7473	°C		
UA	57.57727176	kW/C		
U	35	W/m^2C		
A	1645.064907	m^2		
Type U	Gases to Gases			

Table H16 Sizing equipment of IL process in ethanol + hexane mixture using [EMIM][BTI] (Continued)

Flash drum				
Topic	**V-1**	**Unit**		
type	Vertical			
Pressure	101.3	kPa		
Diameter	3	m		
Height	12	m		

Table H17 Purchase equipment cost calculation of IL process in ethanol + hexane mixture using [EMIM][BTI]

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST
T-1	Tower Unit	9.66	meters	316 Stainless Steel	$ 282,296.00
tT-1	Valve tray	5	trays	Stainless Steel	$ 64,554.00
rT-1	Heat Exchanger	153.758	sq.meter	316 Stainless Steel	$ 46,133.00
cT-1	Heat Exchanger	0.84216	sq.meter	316 Stainless Steel	$ 6,039.00
P-1	Pump	0.01129	cubic meter/s	Stainless Steel	$ 12,739.00
P-2	Pump	0.07882	cubic meter/s	Stainless Steel	$ 26,913.00
M-1	Mixer	0.078819998	cubic meters	Stainless Steel	$ 8,970.00
E-1	Heat Exchanger	45.822	sq.meter	316 Stainless Steel	$ 17,328.00
E-2	Heat Exchanger	28.283	sq.meter	316 Stainless Steel	$ 12,647.00
E-3	Heat Exchanger	111.258	sq.meter	316 Stainless Steel	$ 34,791.00
E-4	Heat Exchanger	1645.065	sq.meter	316 Stainless Steel	$ 174,562.00
E-5	Heat Exchanger	148.237	sq.meter	316 Stainless Steel	$ 44,659.00
V-1	Vessel	10.32	meters	316 Stainless Steel	$ 193,464.00
				Total	**$ 925,095.00**

Table H18 Utility cost calculation of IL process in ethanol + hexane mixture using [EMIM][BTI]

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST
T-1	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-1	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-1	Heat Exchanger	LP steam	6470.19	kW	0.01	$ 2,464.00
cT-1	Heat Exchanger	Cooling water	13584.3	kW	3.769999981	$ 1,326,732.00
P-1	Pump	n/a	n/a	n/a	n/a	$ -
P-2	Pump	n/a	n/a	n/a	n/a	$ -
M-1	Mixer	Electricity	0	kW	23.25	$ -
E-1	Heat Exchanger	Cooling water	1945.9	kW	3.769999981	$ 190,049.00
E-2	Heat Exchanger	LP steam	1638	kW	0.01	$ 624.00
E-3	Heat Exchanger	Cooling water	660.9	kW	3.769999981	$ 64,548.00
E-4	Heat Exchanger	Natural gas	13285.8	kW	1177.29	$ 1,297,578.00
E-5	Heat Exchanger	LP steam	13285.8	kW	0.01	$ 5,059.00
V-1	Vessel	n/a	n/a	n/a	n/a	$ -
					Total	**$ 2,887,054.00**

Table H19 CAPEX calculation of IL process in ethanol + hexane mixture using [EMIM][BTI]

Purchase Equipment Cost	**$ 925,095.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 1,017,604.50
Purchased Equipment Installation	0.47	$ 478,274.12
Instrumentation and Controls (installed)	0.36	$ 366,337.62
Piping (Installed)	0.68	$ 691,971.06
Electrical Systems (Installed)	0.11	$ 111,936.50
Buildings (Including Services)	0.18	$ 183,168.81
Yard Improvement	0.1	$ 101,760.45
Service Facilities (Installed)	0.7	$ 712,323.15
	Total Direct Cost	$ 3,663,376.20

Table H19 CAPEX calculation of IL process in ethanol + hexane mixture using [EMIM][BTI] (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Engineering and Supervision	0.33	$ 335,809.49
Construction Expenses	0.41	$ 417,217.85
Legal Expenses	0.04	$ 40,704.18
Contractor's Fees	0.22	$ 223,872.99
Contingency	0.44	$ 447,745.98
	Total indirect cost	$ 1,465,350.48
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Fixed-capital Investment (FCI)		$ 5,128,726.68
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Working Capital Investment (WC)	0.89	$ 20,352.09
CAPEX	**Total Capital Investment (TCI)**	**$ 5,149,078.77**

Table H20 OPEX calculation of IL process in ethanol + hexane mixture using [EMIM][BTI]

Fixed Capital Investment		**$ 5,128,726.68**	
Plant Capacity		**11724793.92**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 769,309.06
Operating Supervision	0.15	Operating Labor	$ 115,396.36
Utilities	0		$ 2,887,054.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 307,723.62
Operating Supplies	0.15	Maintenance and Supplies	$ 46,158.54
Laboratory Charges	0.15	Operating Labor	$ 115,396.36
Royalties	0.01	Total Product Cost	$ 48,464.68
		Variable Cost	$ 4,289,502.63
Property Taxes	0.02	Fixed Capital Investment	$ 102,574.54
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 51,287.27
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 153,861.81

Table H20 OPEX calculation of IL process in ethanol + hexane mixture using [EMIM][BTI] (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenace	$ 715,457.40
		Manufacturing Cost	$ 4,443,364.44
Administration	0.2	Labor + Supervision + Maintenace	$ 238,485.80
Distribution & selling	0.04	Total Product Cost	$ 193,858.72
Research & Development	0.04	Total Product Cost	$ 193,858.72
		General Expense	$ 626,203.24
OPEX	**Total Product Cost with Out Depreciation**		**$ 4,846,468.00**

Table H21 Sizing equipment of CS process in benzene + hexane mixture using NMP

Sizing equipment of CS process in benzene + hexane mixture using NMP				
Column				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	3	m	4	m
Pressure	100	kPa	100	kPa
Material	316 SS		316 SS	
Number	17	stages	8	stages
Height	15.76	m	10.27	m
Tray				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	2.8	m	3.7	m
Number	15	trays	6	trays
Material	316 SS		316 SS	
Type	valve tray		valve tray	
Spacing	0.61 m	m	0.61 m	m
Condenser				
Topic	**T1**	**Unit**	**T2**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	-4.2086	MMWATT	-8.0091	MMWATT
Stream in	68.5	^{o}C	36.95	^{o}C
Stream out	68.3	^{o}C	35.35	^{o}C
utility	CW		CW	
in	25	^{o}C	25	^{o}C
out	45	^{o}C	35	^{o}C
LMTD	32.39782095	^{o}C	5.032480024	^{o}C
UA	0.129903798	kW/C	1.591481727	kW/C
U	500	W/m^{2}C	500	W/m^{2}C

Table H21 Sizing equipment of CS process in benzene + hexane mixture using NMP (Continued)

Condenser				
Topic	**T1**	**Unit**	**T2**	**Unit**
A	0.259807597	m^2	3.182963454	m^2
Type U	Water to organic vapors		Water to organic vapors	
Reboiler				
Topic	**T1**	**Unit**	**T2**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	8.9626	MMWATT	8.1298	MMWATT
Stream in	97.7	°C	145.25	°C
Stream out	111.9	°C	146.85	°C
utility	LPS		LPS	
in	160	°C	160	°C
out	160	°C	160	°C
LMTD	-54.89423706	°C	-13.93469385	°C
UA	163.2703264	kW/C	583.4215007	kW/C
U	750	W/m^2C	750	W/m^2C
A	217.6937685	m^2	777.8953343	m^2
Type U	Steam to light organic		Steam to light organic	
Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa
Flowrate	54689.23	kg/hr	128819.05	kg/hr
Capacity	0.0172	m3/s	0.0346	m3/s

Table H21 Sizing equipment of CS process in benzene + hexane mixture using NMP (Continued)

Mixer				
Topic	**M-1**	**Unit**		**Unit**
Material	316 SS			
Capacity	0.0346	m3/s		
Heat exchanger				
Topic	**E2**	**Unit**	**E3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	1.8836	MMWATT	0.6636	MMWATT
Stream in	25	°C	68.345	°C
Stream out	68	°C	30	°C
utility	LPS		CW	
LMTD	71.8316	°C	11.905	°C
UA	26.22244249	kW/C	55.74128517	kW/C
U	750	W/m^2C	500	W/m^2C
A	34.96325665	m^2	111.4825703	m^2
Type U	Steam to organic solvents		Water to organic solvents	
Topic	**E1**	**Unit**	**E4**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	5.7361	MMWATT	0.1378	MMWATT
Stream in	146.451	°C	35.35	°C
Stream out	68	°C	30	°C

Table H21 Sizing equipment of CS process in benzene + hexane mixture using NMP (Continued)

Heat exchanger				
Topic	**E1**	**Unit**	**E4**	**Unit**
utility	CW		CW	
LMTD	68.0943	^{o}C	5.1731	^{o}C
UA	84.23759404	kW/C	26.63779939	kW/C
U	500	W/m^2C	500	W/m^2C
A	168.4751881	m^2	53.27559877	m^2
Type U	Water to organic solvents		Water to organic solvents	

Table H22 Purchase equipment cost calculation of CS process in benzene + hexane mixture using NMP

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST	
T-1	Tower Unit	15.76	meters	316 Stainless Steel	$	416,050.00
tT-1	Valve tray	15	trays	Stainless Steel	$	112,466.00
rT-1	Heat Exchanger	217.693	sq.meter	316 Stainless Steel	$	63,195.00
cT-1	Heat Exchanger	0.2598	sq.meter	316 Stainless Steel	$	6,039.00
T-2	Tower Unit	10.27	meters	316 Stainless Steel	$	365,368.00
tT-2	Valve tray	6	trays	Stainless Steel	$	136,379.00
rT-2	Heat Exchanger	777.895	sq.meter	316 Stainless Steel	$	174,562.00
cT-2	Heat Exchanger	3.183	sq.meter	316 Stainless Steel	$	6,039.00
P-1	Pump	0.0172	cubic meter/s	Stainless Steel	$	14,980.00
P-2	Pump	0.0346	cubic meter/s	Stainless Steel	$	19,604.00
M-1	Mixer	0.034600001	cubic meters	Stainless Steel	$	8,970.00
E-1	Heat Exchanger	168.475	sq.meter	316 Stainless Steel	$	50,060.00
E-2	Heat Exchanger	34.963	sq.meter	316 Stainless Steel	$	14,430.00
E-3	Heat Exchanger	111.483	sq.meter	316 Stainless Steel	$	34,851.00
E-4	Heat Exchanger	53.276	sq.meter	316 Stainless Steel	$	19,317.00
				Total	**$**	**1,442,310.00**

Table H23 Utility cost calculation of CS process in benzene + hexane mixture using NMP

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST
T-1	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-1	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-1	Heat Exchanger	LP steam	8962.6	kW	0.01	$ 3,413.00
cT-1	Heat Exchanger	Cooling water	4208.6	kW	3.769999981	$ 411,039.00
T-2	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-2	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-2	Heat Exchanger	LP steam	8129.8	kW	0.01	$ 3,096.00
cT-2	Heat Exchanger	Cooling water	8009.1	kW	3.769999981	$ 782,221.00
P-1	Pump	n/a	n/a	n/a	n/a	$ -
P-2	Pump	n/a	n/a	n/a	n/a	$ -
M-1	Mixer	Electricity	0	kW	23.25	$ -
E-1	Heat Exchanger	Cooling water	5736.1	kW	3.769999981	$ 560,225.00
E-2	Heat Exchanger	LP steam	1883.6	kW	0.01	$ 717.00
E-3	Heat Exchanger	Cooling water	663.6	kW	3.769999981	$ 64,812.00
E-4	Heat Exchanger	Cooling water	137.8	kW	3.769999981	$ 13,458.00
					Total	**$ 1,838,981.00**

Table H24 CAPEX calculation of CS process in benzene + hexane mixture using NMP

Purchase Equipment Cost	**$ 1,442,310.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 1,586,541.00
Purchased Equipment Installation	0.47	$ 745,674.27
Instrumentation and Controls (installed)	0.36	$ 571,154.76
Piping (Installed)	0.68	$ 1,078,847.88
Electrical Systems (Installed)	0.11	$ 174,519.51
Buildings (Including Services)	0.18	$ 285,577.38
Yard Improvement	0.1	$ 158,654.10
Service Facilities (Installed)	0.7	$ 1,110,578.70
	Total Direct Cost	$ 5,711,547.60

Table H24 CAPEX calculation of CS process in benzene + hexane mixture using NMP (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Engineering and Supervision	0.33	$ 523,558.53
Construction Expenses	0.41	$ 650,481.81
Legal Expenses	0.04	$ 63,461.64
Contractor's Fees	0.22	$ 349,039.02
Contingency	0.44	$ 698,078.04
	Total indirect cost	$ 2,284,619.04
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Fixed-capital Investment (FCI)		$ 7,996,166.64
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result
Working Capital Investment (WC)	0.89	$ 31,730.82
CAPEX	**Total Capital Investment (TCI)**	**$ 8,027,897.46**

Table H25 OPEX calculation of CS process in benzene + hexane mixture using NMP

Fixed Capital Investment		**$ 7,996,166.64**	
Plant Capacity		**5031866.9**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 1,199,425.00
Operating Supervision	0.15	Operating Labor	$ 179,913.75
Utilities	0		$ 1,838,981.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 479,770.02
Operating Supplies	0.15	Maintenance and Supplies	$ 71,965.50
Laboratory Charges	0.15	Operating Labor	$ 179,913.75
Royalties	0.01	Total Product Cost	$ 46,305.96
		Variable Cost	$ 3,996,274.98
Property Taxes	0.02	Fixed Capital Investment	$ 159,923.34
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 79,961.67
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 239,885.01

Table H25 OPEX calculation of CS process in benzene + hexane mixture using NMP (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenace	$ 1,115,465.25
		Manufacturing Cost	$ 4,236,159.99
Administration	0.2	Labor + Supervision + Maintenace	$ 371,821.75
Distribution & selling	0.04	Total Product Cost	$ 185,223.84
Research & Development	0.04	Total Product Cost	$ 185,223.84
		General Expense	$ 742,269.43
OPEX	**Total Product Cost with Out Depreciation**		**$ 4,630,596.00**

Table H26 Sizing equipment of IL process in benzene + hexane mixture using [EMIM][EtSO4]

Sizing equipment of IL process in benzene + hexane mixture using [EMIM][EtSO4]				
Column				
Topic	**T1**	**Unit**		
Diameter	3	m		
Pressure	100	kPa		
Material	316 SS			
Number	17	stages		
Height	15.76	m		
Tray				
Topic	**T1**	**Unit**		
Diameter	3	m		
Number	15	trays		
Material	316 SS			
Type	valve tray			
Spacing	0.61 m	m		
Condenser				
Topic	**T1**	**Unit**		
Type	Shell & Tube			
Material	316 SS			
Duty	-3.3017	MMWATT		
Stream in	68.3	^{o}C		
Stream out	68.3	^{o}C		
utility	CW			
in	25	^{o}C		
out	45	^{o}C		

Table H26 Sizing equipment of IL process in benzene + hexane mixture using [EMIM][EtSO4] (Continued)

Condenser				
Topic	**T1**	**Unit**		
LMTD	32.2737186	°C		
UA	0.102303055	kW/C		
U	500	W/m^2C		
A	0.204606109	m^2		
Type U	Water to organic vapors			
Reboiler				
Topic	**T1**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	3.421	MMWATT		
Stream in	70.7	°C		
Stream out	76.3	°C		
utility	LPS			
in	160	°C		
out	160	°C		
LMTD	-86.46977961	°C		
UA	39.56295501	kW/C		
U	750	W/m^2C		
A	52.75060667	m^2		
Type U	Steam to light organic			

Table H26 Sizing equipment of IL process in benzene + hexane mixture using [EMIM][EtSO4] (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa
Flowrate	54645.202	kg/hr	94530.994	kg/hr
Capacity	0.0172	m3/s	0.0212	m3/s
Mixer				
Topic	M-1	**Unit**		**Unit**
Material	316 SS			
Capacity	0.0212	m3/s		
Heat exchanger				
Topic	**E-2**	**Unit**	**E-3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	1.8836	MMWATT	0.6625	MMWATT
Stream in	25	^{o}C	68.314	^{o}C
Stream out	68	^{o}C	30	^{o}C
utility	LPS		CW	
LMTD	71.8316	^{o}C	11.8951	^{o}C
UA	26.22244249	kW/C	55.69520223	kW/C
U	750	W/m^2C	500	W/m^2C
A	34.96325665	m^2	111.3904045	m^2
Type U	Steam to organic solvents		Water to organic solvents	

Table H26 Sizing equipment of IL process in benzene + hexane mixture using [EMIM][EtSO4] (Continued)

Heat exchanger				
Topic	**E-1**	**Unit**	**E-5**	**Unit**
type	Shell & Tube		Shell & Tube	
utility	CW		LPS	
LMTD	39.0643	°C	126.7206	°C
UA	1.776558136	kW/C	14.62824513	kW/C
U	500	W/m^2C	750	W/m^2C
A	3.553116272	m^2	19.50432684	m^2
Type U	Water to organic solvents		Steam to organic solvents	
Topic	**E-4**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	9.1892	MMWATT		
Stream in	80.3	°C		
Stream out	-51.128	°C		
utility	NG			
LMTD	167.7344	°C		
UA	54.78423031	kW/C		
U	35	W/m^2C		
A	1565.263723	m^2		
Type U	Gases to Gases			
Flash drum				
Topic	**V-1**	**Unit**		
type	Vertical			
Pressure	101.3	kPa		
Diameter	2	m		
Height	8	m		

Table H27 Purchase equipment cost calculation of IL process in benzene + hexane mixture using [EMIM][EtSO4]

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST
T-1	Tower Unit	15.76	meters	316 Stainless Steel	$ 416,050.00
tT-1	Valve tray	15	trays	Stainless Steel	$ 112,466.00
rT-1	Heat Exchanger	52.7506	sq.meter	316 Stainless Steel	$ 19,177.00
cT-1	Heat Exchanger	0.2046	sq.meter	316 Stainless Steel	$ 6,039.00
P-1	Pump	0.0172	cubic meter/s	Stainless Steel	$ 14,980.00
P-2	Pump	0.0212	cubic meter/s	Stainless Steel	$ 16,235.00
M-1	Mixer	0.021199999	cubic meters	Stainless Steel	$ 8,970.00
E-1	Heat Exchanger	3.553	sq.meter	316 Stainless Steel	$ 6,048.00
E-2	Heat Exchanger	34.963	sq.meter	316 Stainless Steel	$ 14,430.00
E-3	Heat Exchanger	111.39	sq.meter	316 Stainless Steel	$ 34,826.00
E-4	Heat Exchanger	1565	sq.meter	316 Stainless Steel	$ 174,562.00
E-5	Heat Exchanger	19.504	sq.meter	316 Stainless Steel	$ 10,304.00
V-1	Vessel	8	meters	316 Stainless Steel	$ 157,516.00
				Total	**$ 991,603.00**

Table H28 Utility cost calculation of IL process in benzene + hexane mixture using [EMIM][EtSO4]

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST
T-1	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-1	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-1	Heat Exchanger	LP steam	3421	kW	0.01	$ 1,303.00
cT-1	Heat Exchanger	Cooling water	3301.7	kW	3.769999981	$ 322,466.00
P-1	Pump	n/a	n/a	n/a	n/a	$ -
P-2	Pump	n/a	n/a	n/a	n/a	$ -
M-1	Mixer	Electricity	0	kW	23.25	$ -
E-1	Heat Exchanger	Cooling water	69.4	kW	3.769999981	$ 6,778.00
E-2	Heat Exchanger	LP steam	1883.6	kW	0.01	$ 717.00
E-3	Heat Exchanger	Cooling water	662.5	kW	3.769999981	$ 64,704.00
E-4	Heat Exchanger	Natural gas	9189.2	kW	1177.29	$ 897,478.00
E-5	Heat Exchanger	LP steam	1853.7	kW	0.01	$ 706.00
V-1	Vessel	n/a	n/a	n/a	n/a	$ -
					Total	**$ 1,294,152.00**

Table H29 CAPEX calculation of IL process in benzene + hexane mixture using [EMIM][EtSO4]

Purchase Equipment Cost	**$ 991,603.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 1,090,763.30
Purchased Equipment Installation	0.47	$ 512,658.75
Instrumentation and Controls (installed)	0.36	$ 392,674.79
Piping (Installed)	0.68	$ 741,719.04
Electrical Systems (Installed)	0.11	$ 119,983.96
Buildings (Including Services)	0.18	$ 196,337.39
Yard Improvement	0.1	$ 109,076.33
Service Facilities (Installed)	0.7	$ 763,534.31
	Total Direct Cost	$ 3,926,747.88

Table H29 CAPEX calculation of IL process in benzene + hexane mixture using [EMIM][EtSO4] (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Engineering and Supervision	0.33	$	359,951.89
Construction Expenses	0.41	$	447,212.95
Legal Expenses	0.04	$	43,630.53
Contractor's Fees	0.22	$	239,967.93
Contingency	0.44	$	479,935.85
	Total indirect cost	$	1,570,699.15
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Fixed-capital Investment (FCI)		$	5,497,447.03
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Working Capital Investment (WC)	0.89	$	21,815.27
CAPEX	**Total Capital Investment (TCI)**	**$**	**5,519,262.30**

Table H30 OPEX calculation of IL process in benzene + hexane mixture using [EMIM][EtSO4]

Fixed Capital Investment		**$ 5,497,447.03**	
Plant Capacity		**5031866.9**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.150000006	Fixed Capital Investment	$ 824,617.06
Operating Supervision	0.15	Operating Labor	$ 123,692.56
Utilities	0		$ 1,294,152.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 329,846.82
Operating Supplies	0.15	Maintenance and Supplies	$ 49,477.02
Laboratory Charges	0.15	Operating Labor	$ 123,692.56
Royalties	0.01	Total Product Cost	$ 32,163.67
		Variable Cost	$ 2,777,641.69
Property Taxes	0.02	Fixed Capital Investment	$ 109,948.94
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 54,974.47
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 164,923.41

Table H30 OPEX calculation of IL process in benzene + hexane mixture using [EMIM][EtSO4] (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenace	$ 766,893.90
		Manufacturing Cost	$ 2,942,565.10
Administration	0.2	Labor + Supervision + Maintenace	$ 255,631.30
Distribution & selling	0.04	Total Product Cost	$ 128,654.67
Research & Development	0.04	Total Product Cost	$ 128,654.67
		General Expense	$ 512,940.64
OPEX	**Total Product Cost with Out Depreciation**		**$ 3,216,366.75**

Table H31 Sizing equipment of CS process in toluene + MCH mixture using NMP

Sizing equipment of CS process in toluene + MCH mixture using NMP				
Column				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	4	m	4	m
Pressure	100	kPa	100	kPa
Material	316 SS		316 SS	
Number	30	stages	15	stages
Height	23.69 m	m	13.93	m
Tray				
Topic	**T1**	**Unit**	**T2**	**Unit**
Diameter	4	m	4	m
Number	28	trays	13	trays
Material	316 SS		316 SS	
Type	valve tray		valve tray	
Spacing	0.61 m	m	0.61 m	m
Condenser				
Topic	**T1**	**Unit**	**E-D1**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	-10.0201	MMWATT	-10.5493	MMWATT
Stream in	100.4	^{o}C	80.9	^{o}C
Stream out	100.4	^{o}C	80.9	^{o}C
utility	CW		CW	
in	25	^{o}C	25	^{o}C
out	45	^{o}C	45	^{o}C
LMTD	64.88709878	^{o}C	45.16435578	^{o}C
UA	0.154423609	kW/C	0.233575788	kW/C
U	500	W/m^2C	500	W/m^2C

Table H31 Sizing equipment of CS process in toluene + MCH mixture using NMP (Continued)

Condenser				
Topic	**T1**	**Unit**	**E-D1**	**Unit**
A	0.308847219	m^2	0.467151576	m^2
Type U	Water to organic vapors		Water to organic vapors	
Reboiler				
Topic	**T1**	**Unit**	**E-D1**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	13.8969	MMWATT	11.3257	MMWATT
Stream in	119.4	°C	166.9	°C
Stream out	131.7	°C	167.8	°C
utility	LPS		LPS	
in	160	°C	160	°C
out	160	°C	160	°C
LMTD	-34.08087167	°C	7.340807129	°C
UA	407.7624579	kW/C	1542.841244	kW/C
U	750	W/m^2C	750	W/m^2C
A	543.6832772	m^2	2057.121658	m^2
Type U	Steam to light organic		Steam to light organic	

Table H31 Sizing equipment of CS process in toluene + MCH mixture using NMP (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa
Flowrate	64507.86	kg/hr	135844.73	kg/hr
Capacity	0.0205	m3/s	0.0365	m3/s
Mixer				
Topic	M-1	**Unit**		**Unit**
Material	316 SS			
Capacity	0.0365	m3/s		
Heat exchanger				
Topic	**E2**	**Unit**	**E3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	3.8269	MMWATT	1.2044	MMWATT
Heat exchanger				
Topic	**E2**	**Unit**	**E3**	**Unit**
Stream in	25	^{o}C	100.371	^{o}C
Stream out	101	^{o}C	30	^{o}C
utility	LPS		CW	
LMTD	83.375	^{o}C	20.948	^{o}C
UA	45.89985007	kW/C	57.4947489	kW/C
U	750	W/m^2C	500	W/m^2C
A	61.1998001	m^2	114.9894978	m^2
Type U	Steam to organic solvents		Water to organic solvents	

Table H31 Sizing equipment of CS process in toluene + MCH mixture using NMP (Continued)

Topic	E1	Unit	E4	Unit
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	5.3954	MMWATT	1.6745	MMWATT
Stream in	167.8	°C	80.879	°C
Stream out	101	°C	30	°C
utility	CW		CW	
LMTD	97.325	°C	15.669	°C
UA	55.43693809	kW/C	106.8670624	kW/C
U	500	W/m^2C	500	W/m^2C
A	110.8738762	m^2	213.7341247	m^2
Type U	Water to organic solvents		Water to organic solvents	

Table H32 Purchase equipment cost calculation of CS process in toluene + MCH mixture using NMP

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST
T-1	Tower Unit	23.69	meters	316 Stainless Steel	$ 681,213.00
tT-1	Valve tray	28	trays	Stainless Steel	$ 278,736.00
rT-1	Heat Exchanger	543.683	sq.meter	316 Stainless Steel	$ 150,192.00
cT-1	Heat Exchanger	0.3088	sq.meter	316 Stainless Steel	$ 6,039.00
T-2	Tower Unit	13.93	meters	316 Stainless Steel	$ 452,369.00
tT-2	Valve tray	13	trays	Stainless Steel	$ 164,389.00
rT-2	Heat Exchanger	2057.122	sq.meter	316 Stainless Steel	$ 174,562.00
cT-2	Heat Exchanger	0.4672	sq.meter	316 Stainless Steel	$ 6,039.00
P-1	Pump	0.0205	cubic meter/s	Stainless Steel	$ 16,027.00
P-2	Pump	0.0365	cubic meter/s	Stainless Steel	$ 20,011.00
M-1	Mixer	0.036499999	cubic meters	Stainless Steel	$ 8,970.00
E-1	Heat Exchanger	110.8739	sq.meter	316 Stainless Steel	$ 34,688.00
E-2	Heat Exchanger	61.3597	sq.meter	316 Stainless Steel	$ 21,474.00
E-3	Heat Exchanger	114.9895	sq.meter	316 Stainless Steel	$ 35,787.00
E-4	Heat Exchanger	213.7341	sq.meter	316 Stainless Steel	$ 62,139.00
				Total	**$ 2,112,635.00**

Table H33 Utility cost calculation of CS process in toluene + MCH mixture using NMP

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST	
T-1	Tower Unit	n/a	n/a	n/a	n/a	$	-
tT-1	Valve tray	n/a	n/a	n/a	n/a	$	-
rT-1	Heat Exchanger	LP steam	13896.9	kW	0.01	$	5,291.00
cT-1	Heat Exchanger	Cooling water	10020.1	kW	3.769999981	$	978,629.00
T-2	Tower Unit	n/a	n/a	n/a	n/a	$	-
tT-2	Valve tray	n/a	n/a	n/a	n/a	$	-
rT-2	Heat Exchanger	LP steam	11325.7	kW	0.01	$	4,312.00
cT-2	Heat Exchanger	Cooling water	10549.3	kW	3.769999981	$	1,030,314.00
P-1	Pump	n/a	n/a	n/a	n/a	$	-
P-2	Pump	n/a	n/a	n/a	n/a	$	-
M-1	Mixer	Electricity	0	kW	23.25	$	-
E-1	Heat Exchanger	Cooling water	5395.4	kW	3.769999981	$	526,950.00
E-2	Heat Exchanger	LP steam	3826.9	kW	0.01	$	1,457.00
E-3	Heat Exchanger	Cooling water	1204.4	kW	3.769999981	$	117,630.00
E-4	Heat Exchanger	Cooling water	1674.5	kW	3.769999981	$	163,543.00
					Total	**$**	**2,828,126.00**

Table H34 CAPEX calculation of CS process in toluene + MCH mixture using NMP

Purchase Equipment Cost	**$ 2,112,635.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 2,323,898.50
Purchased Equipment Installation	0.47	$ 1,092,232.30
Instrumentation and Controls (installed)	0.36	$ 836,603.46
Piping (Installed)	0.68	$ 1,580,250.98
Electrical Systems (Installed)	0.11	$ 255,628.84
Buildings (Including Services)	0.18	$ 418,301.73
Yard Improvement	0.1	$ 232,389.85
Service Facilities (Installed)	0.7	$ 1,626,728.95
	Total Direct Cost	$ 8,366,034.60

Table H34 CAPEX calculation of CS process in toluene + MCH mixture using NMP (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Engineering and Supervision	0.33	$	766,886.51
Construction Expenses	0.41	$	952,798.39
Legal Expenses	0.04	$	92,955.94
Contractor's Fees	0.22	$	511,257.67
Contingency	0.44	$	1,022,515.34
	Total indirect cost	$	3,346,413.84
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Fixed-capital Investment (FCI)		$	11,712,448.44
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Working Capital Investment (WC)	0.89	$	46,477.97
CAPEX	**Total Capital Investment (TCI)**	**$**	**11,758,926.41**

Table H35 OPEX calculation of CS process in toluene + MCH mixture using NMP

Fixed Capital Investment		**$ 11,712,448.44**	
Plant Capacity		**5520916.93**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 1,756,867.38
Operating Supervision	0.15	Operating Labor	$ 263,530.11
Utilities	0		$ 2,828,126.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 702,746.88
Operating Supplies	0.15	Maintenance and Supplies	$ 105,412.03
Laboratory Charges	0.15	Operating Labor	$ 263,530.11
Royalties	0.01	Total Product Cost	$ 92,858.25
		Variable Cost	$ 6,013,070.75
Property Taxes	0.02	Fixed Capital Investment	$ 234,248.96
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 117,124.48
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 351,373.44

Table H35 OPEX calculation of CS process in toluene + MCH mixture using NMP (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenance	$ 1,633,886.55
		Manufacturing Cost	$ 6,364,444.19
Administration	0.2	Labor + Supervision + Maintenance	$ 544,628.85
Distribution & selling	0.04	Total Product Cost	$ 371,433.00
Research & Development	0.04	Total Product Cost	$ 371,433.00
		General Expense	$ 1,287,494.85
OPEX	**Total Product Cost with Out Depreciation**		**$ 9,285,825.00**

Table H36 Sizing equipment of IL process in toluene + MCH mixture using [HMIM][TCB]

Sizing equipment of IL process in toluene + MCH mixture using [HMIM][TCB]				
Column				
Topic	**T1**	**Unit**		
Diameter	4	m		
Pressure	100	kPa		
Material	316 SS			
Number	30	stages		
Height	23.69 m	m		
Tray				
Topic	**T1**	**Unit**		
Diameter	4	m		
Number	28	trays		
Material	316 SS			
Type	valve tray			
Spacing	0.61 m	m		
Condenser				
Topic	**T1**	**Unit**		
Type	Shell & Tube			
Material	316 SS			
Duty	-7.9235	MMWATT		
Stream in	100.3	^{o}C		
Stream out	100.3	^{o}C		
utility	CW			
in	25	^{o}C		
out	45	^{o}C		
LMTD	64.78630332	^{o}C		

Table H36 Sizing equipment of IL process in toluene + MCH mixture using [HMIM][TCB] (Continued)

Condenser				
Topic	**T1**	**Unit**		
UA	0.122302085	kW/C		
U	500	W/m^2C		
A	0.244604171	m^2		
Type U	Water to organic vapors			
Reboiler				
Topic	**T1**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	13.8969	MMWATT		
Stream in	110.6	°C		
Stream out	110.7	°C		
utility	LPS			
in	160	°C		
out	160	°C		
LMTD	-49.34998311	°C		
UA	281.5988805	kW/C		
U	750	W/m^2C		
A	375.4651741	m^2		
Type U	Steam to light organic			

Table H36 Sizing equipment of IL process in toluene + MCH mixture using [HMIM][TCB] (Continued)

Pump				
Topic	**PD-2**	**Unit**	**PB-2**	**Unit**
Type	centrifugal		centrifugal	
Material	316 SS		316 SS	
Pressure	100	kPa	100	kPa
Flowrate	64437.072	kg/hr	70829.668	kg/hr
Capacity	0.0205	m3/s	0.001989	m3/s
Mixer				
Topic	M-1	**Unit**		**Unit**
Material	316 SS			
Capacity	0.001989	m3/s		
Heat exchanger				
Topic	**E-2**	**Unit**	**E-3**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	3.8269	MMWATT	1.2008	MMWATT
Stream in	25	°C	100.371	°C
Stream out	101	°C	30	°C
utility	LPS		CW	
LMTD	83.375	°C	20.937	°C
UA	45.89985007	kW/C	57.35301142	kW/C
U	750	W/m^2C	500	W/m^2C
A	61.1998001	m^2	114.7060228	m^2
Type U	Steam to organic solvents		Water to organic solvents	

Table H36 Sizing equipment of IL process in toluene + MCH mixture using [HMIM][TCB] (Continued)

Heat exchanger				
Topic	**E-1**	**Unit**	**E-5**	**Unit**
type	Shell & Tube		Shell & Tube	
material	316 SS		316 SS	
Duty	0.4302	MMWATT	1.7239	MMWATT
Stream in	167.8	°C	80.879	°C
Stream out	101	°C	30	°C
utility	CW		LPS	
LMTD	89.289	°C	150.156	°C
UA	4.818062695	kW/C	11.48072671	kW/C
U	500	W/m^2C	750	W/m^2C
A	9.636125391	m^2	15.30763561	m^2
Type U	Water to organic solvents		Steam to organic solvents	
Topic	**E-4**	**Unit**		
type	Shell & Tube			
material	316 SS			
Duty	12.047	MMWATT		
Stream in	149.226	°C		
Stream out	-30.201	°C		
utility	NG			
LMTD	208.442	°C		
UA	57.79545389	kW/C		

Table H36 Sizing equipment of IL process in toluene + MCH mixture using [HMIM][TCB] (Continued)

Heat exchanger				
Topic	**E-4**	**Unit**		
U	35	W/m^2C		
A	1651.298683	m^2		
Type U	Gases to Gases			
Flash drum				
Topic	**V-1**	**Unit**		
type	Vertical			
Pressure	101.3	kPa		
Diameter	2	m		
Height	8	m		

Table H37 Purchase equipment cost calculation of IL process in toluene + MCH mixture using [HMIM][TCB]

No.	EQUIPMENT	SIZE	UNIT	MATERIAL	PURCHASE COST	
T-1	Tower Unit	23.69	meters	316 Stainless Steel	$	681,213.00
tT-1	Valve tray	28	trays	Stainless Steel	$	246,605.00
rT-1	Heat Exchanger	375.465	sq.meter	316 Stainless Steel	$	105,300.00
cT-1	Heat Exchanger	0.2446	sq.meter	316 Stainless Steel	$	6,039.00
P-1	Pump	0.0205	cubic meter/s	Stainless Steel	$	16,027.00
P-2	Pump	0.001989	cubic meter/s	Stainless Steel	$	6,101.00
M-1	Mixer	0.001989	cubic meters	Stainless Steel	$	8,970.00
E-1	Heat Exchanger	9.6361	sq.meter	316 Stainless Steel	$	7,671.00
E-2	Heat Exchanger	61.1998	sq.meter	316 Stainless Steel	$	21,432.00
E-3	Heat Exchanger	114.706	sq.meter	316 Stainless Steel	$	35,711.00
E-4	Heat Exchanger	1651.2987	sq.meter	316 Stainless Steel	$	174,562.00
V-1	Vessel	8	meters	316 Stainless Steel	$	157,516.00
				Total	**$**	**1,467,147.00**

Table H38 Utility cost calculation of IL process in toluene + MCH mixture using [HMIM][TCB]

No.	EQUIPMENT	UTILITY	SIZE	UNIT	PRICE, $/GJ	UTILITY COST
T-1	Tower Unit	n/a	n/a	n/a	n/a	$ -
tT-1	Valve tray	n/a	n/a	n/a	n/a	$ -
rT-1	Heat Exchanger	LP steam	13896.9	kW	0.01	$ 5,291.00
cT-1	Heat Exchanger	Cooling water	7923.5	kW	3.769999981	$ 773,861.00
P-1	Pump	n/a	n/a	n/a	n/a	$ -
P-2	Pump	n/a	n/a	n/a	n/a	$ -
M-1	Mixer	Electricity	0	kW	23.25	$ -
E-1	Heat Exchanger	Cooling water	430.2	kW	3.769999981	$ 42,016.00
E-2	Heat Exchanger	LP steam	3826.9	kW	0.01	$ 1,457.00
E-3	Heat Exchanger	Cooling water	1200.8	kW	3.769999981	$ 117,278.00
E-4	Heat Exchanger	Natural gas	12047	kW	1177.29	$ 1,176,589.00
V-1	Vessel	n/a	n/a	n/a	n/a	$ -
					Total	**$ 2,116,492.00**

Table H39 CAPEX calculation of IL process in toluene + MCH mixture using [HMIM][TCB]

Purchase Equipment Cost	**$ 1,467,147.00**	
Manufacturing Fixed-capital Investment (Direct Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result
Purchased Equipment Delivered	1.1	$ 1,613,861.70
Purchased Equipment Installation	0.47	$ 758,515.00
Instrumentation and Controls (installed)	0.36	$ 580,990.21
Piping (Installed)	0.68	$ 1,097,425.96
Electrical Systems (Installed)	0.11	$ 177,524.79
Buildings (Including Services)	0.18	$ 290,495.11
Yard Improvement	0.1	$ 161,386.17
Service Facilities (Installed)	0.7	$ 1,129,703.19
	Total Direct Cost	$ 5,809,902.12

Table H39 CAPEX calculation of IL process in toluene + MCH mixture using [HMIM][TCB] (Continued)

Nonmanufacturing Fixed-capital Investment (Indirect Cost)	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Engineering and Supervision	0.33	$	532,574.36
Construction Expenses	0.41		
Legal Expenses	0.04	$	64,554.47
Contractor's Fees	0.22	$	355,049.57
Contingency	0.44	$	710,099.15
	Total indirect cost	$	2,323,960.85
Fixed-capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Fixed-capital Investment (FCI)		$	8,133,862.97
Working Capital Investment	Percent of Delivered-equipment for Fluid Processing Plant	Result	
Working Capital Investment (WC)	0.89	$	32,277.23
CAPEX	**Total Capital Investment (TCI)**	**$**	**8,166,140.20**

Table H40 OPEX calculation of IL process in toluene + MCH mixture using [HMIM][TCB]

Fixed Capital Investment		**$ 8,133,862.97**	
Plant Capacity		**8048230.34**	**kg/day**
Items of Operating Cost	**Factor (can change by user)**	**Basis**	**Cost, $/year**
Operating Labor	0.15	Fixed Capital Investment	$ 1,220,079.50
Operating Supervision	0.15	Operating Labor	$ 183,011.93
Utilities	0		$ 2,116,492.00
Maintenance and Repairs	0.06	Fixed Capital Investment	$ 488,031.78
Operating Supplies	0.15	Maintenance and Supplies	$ 73,204.77
Laboratory Charges	0.15	Operating Labor	$ 183,011.93
Royalties	0.01	Total Product Cost	$ 49,804.94
		Variable Cost	$ 4,313,636.84
Property Taxes	0.02	Fixed Capital Investment	$ 162,677.26
Financing (interest)	0	Fixed Capital Investment	$ -
Insurance	0.01	Fixed Capital Investment	$ 81,338.63
Rent	0	Fixed Capital Investment	$ -
		Fixed Charges	$ 244,015.89

Table H40 OPEX calculation of IL process in toluene + MCH mixture using [HMIM][TCB] (Continued)

Items of Operating Cost	Factor (can change by user)	Basis	Cost, $/year
Plant Overhead	0.6	Labor + Supervision + Maintenance	$ 1,134,673.95
		Manufacturing Cost	$ 4,557,652.73
Administration	0.2	Labor + Supervision + Maintenance	$ 378,224.65
Distribution & selling	0.04	Total Product Cost	$ 199,219.76
Research & Development	0.04	Total Product Cost	$ 199,219.76
		General Expense	$ 776,664.17
OPEX	**Total Product Cost with Out Depreciation**		**$ 4,980,494.00**

Appendix I Supplementary Case Study of Ethanol + Heptane Mixture

- Screening graphs of ethanol + heptane mixture (Figure I1 - I2)
- Table of vapor pressure and heat of vaporization of ethanol and heptane (Table I1)
- Graph of vapor pressure of ethanol and heptane (Figure I3)
- Graph of heat of vaporization of ethanol and heptane (Figure I4)
- VLE graph of ethanol + heptane mixture (Figure I5)
- VLE graph of [EMIM]BTI] in ethanol + heptane mixture (Figure I6)
- VLE graph of [BMIM][BTI] in ethanol + heptane mixture (Figure I7)

In the case of ethanol + heptane mixture, I have studied a few additional to observe the flexibility for ethanol series, namely ethanol + hexane and ethanol + heptane mixtures. It is noted that the results from screening graphs of both case studies gave a good agreement, for instance, ethanol was the same as the selected target solute and the same eight feasible IL candidates were screened. Owing to the higher vapor pressure and lower heat of vaporization as shown in Table I1 (or Figures I3 and I4), heptane should be the suitable target solute. In addition, the VLE graph of ethanol + heptane mixture as shown in Figure I3 showed that heptane has a small quantity and commonly should be extracted than ethanol. Nevertheless, the high polar effects of ILs were more influenced with ethanol. Hence, the verification of mixture step has just been the additional data to confirm the target solute from screening criteria. According to VLE graph of [EMIM][BTI] and [BMIM][BTI] in ethanol + heptane mixture as shown in Figure I4 and I5, respectively, the separation capability of both ILs can break azeotrope by extracting ethanol perfectly. It is predicted that the separation process of ILs would be used high energy requirement and solvent usage.

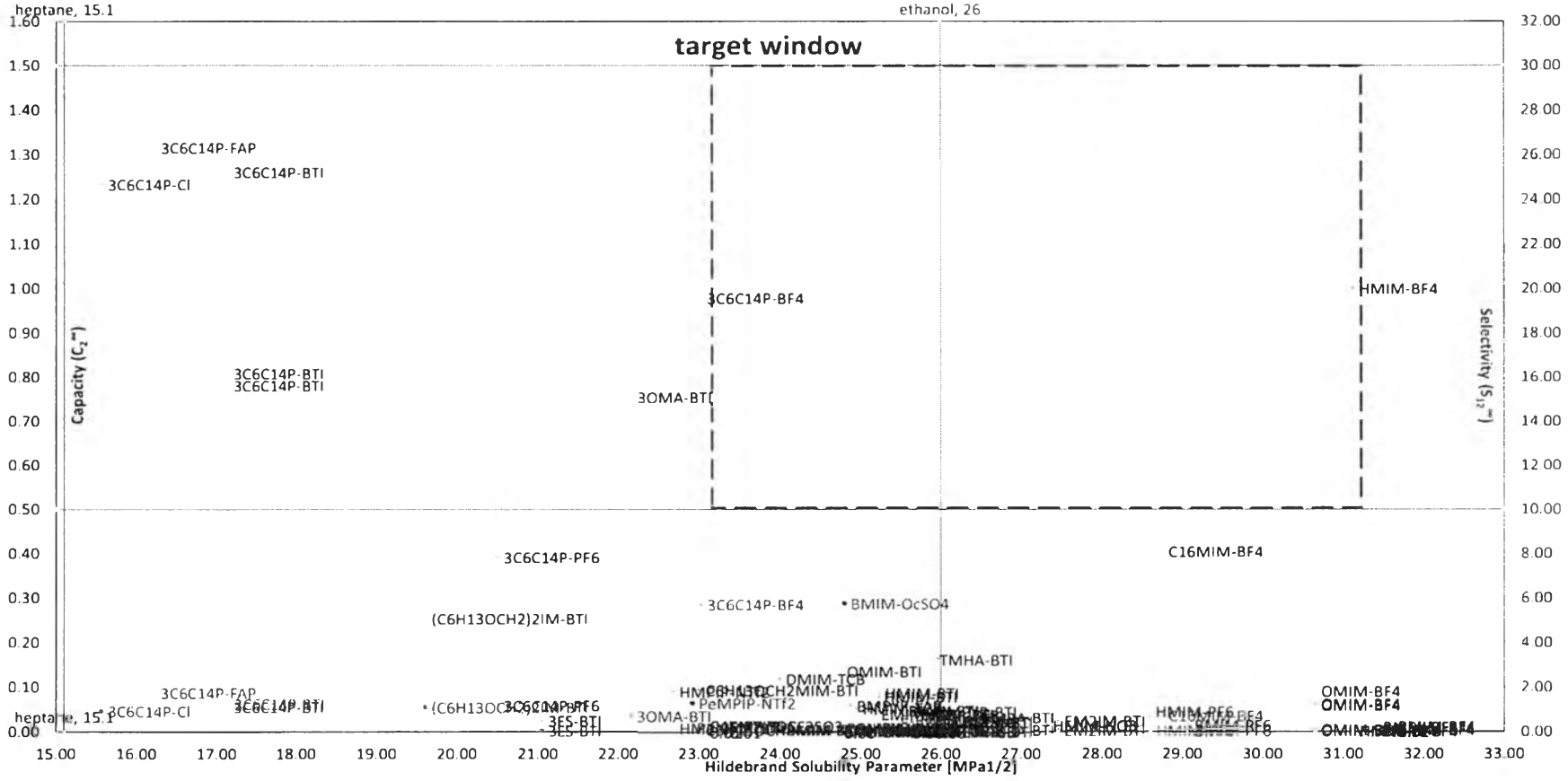

Figure I1 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^{∞}) of ILs (primary *y-axis*) and Selectivity (S_{12}^{∞}) of ILs (secondary *y-axis*) of the ethanol + heptane mixture. Heptane is the target solute.

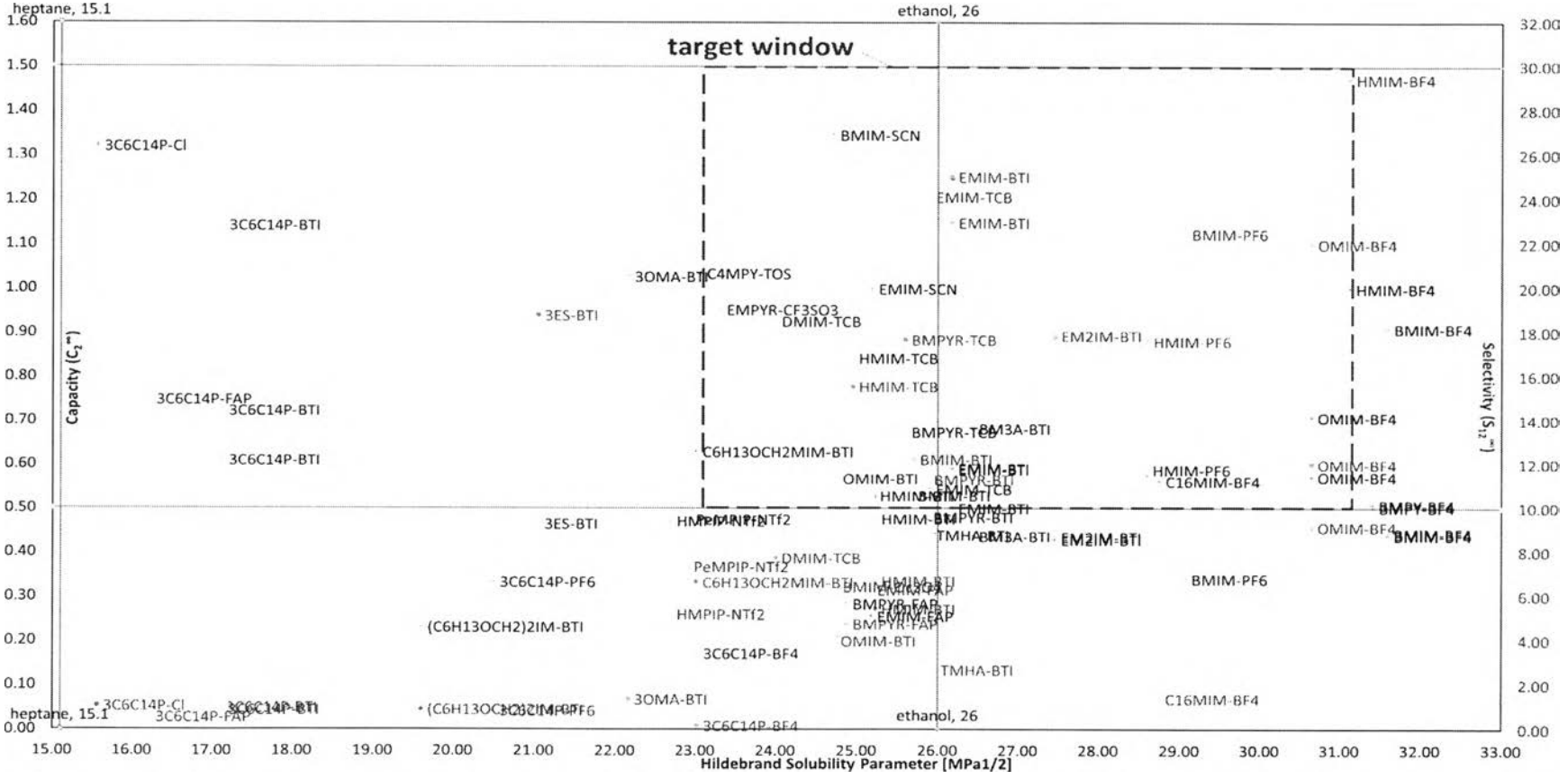

Figure I2 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the ethanol + heptane mixture. Ethanol is the target solute.

Table I1 Vapor pressure and heat of vaporization with various temperature of ethanol + heptane mixture

T (K)	P^0 (kPa)		H_{vap} (kJ/mol)	
	heptane	**ethanol**	**heptane**	**ethanol**
351.35	45.76036	101.542	33.10	38.23
353.35	51.23496	109.92	32.96	38.04
355.35	56.70956	118.8543	32.83	37.85
357.35	62.18416	128.3723	32.69	37.65
359.35	67.65876	138.5019	32.56	37.46
361.35	73.13336	149.2716	32.42	37.27
Comparison	Ethanol > Heptane		Heptane > Ethanol	
Suitable Target solute		Heptane		

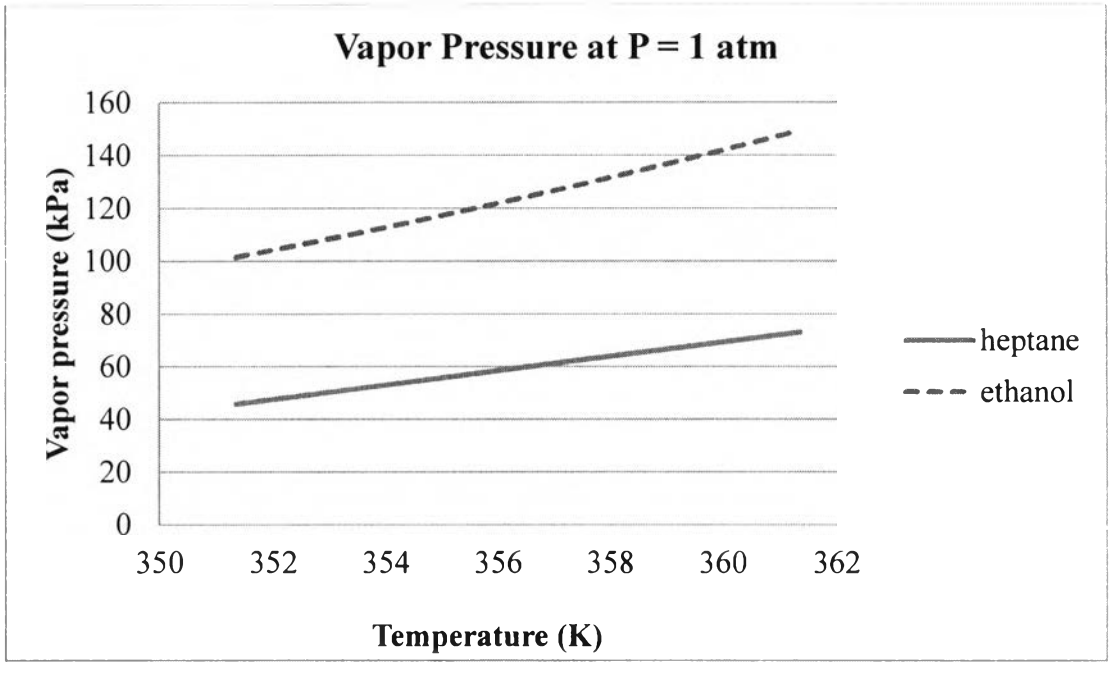

Figure I3 Graph between vapor pressure and temperature with various temperature of ethanol + heptane mixture.

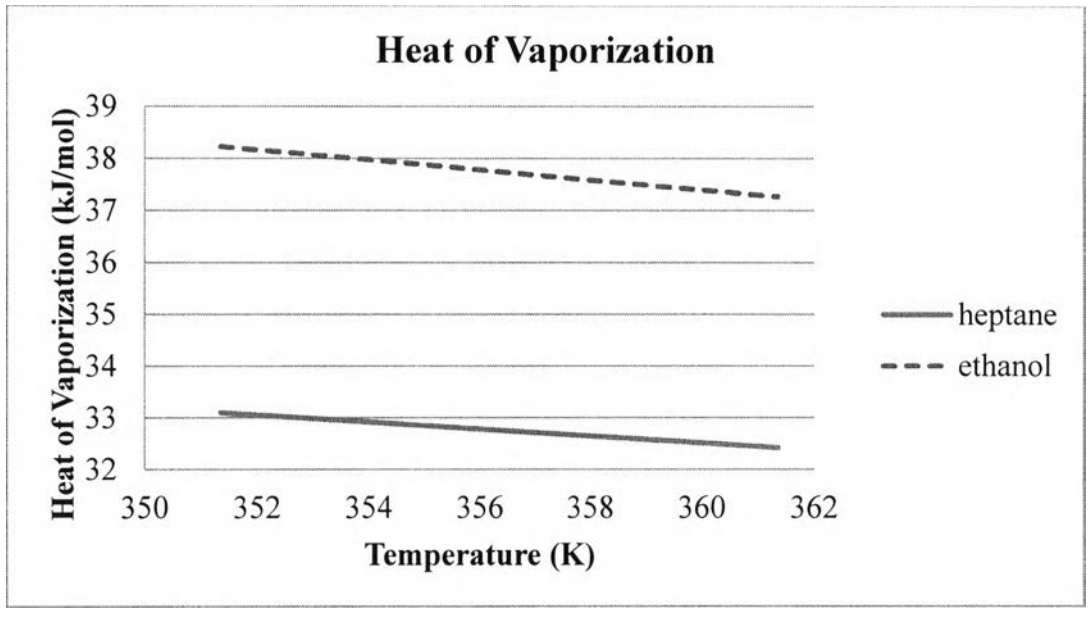

Figure I4 Graph between heat of vaporization and temperature with various temperature of ethanol + heptane mixture.

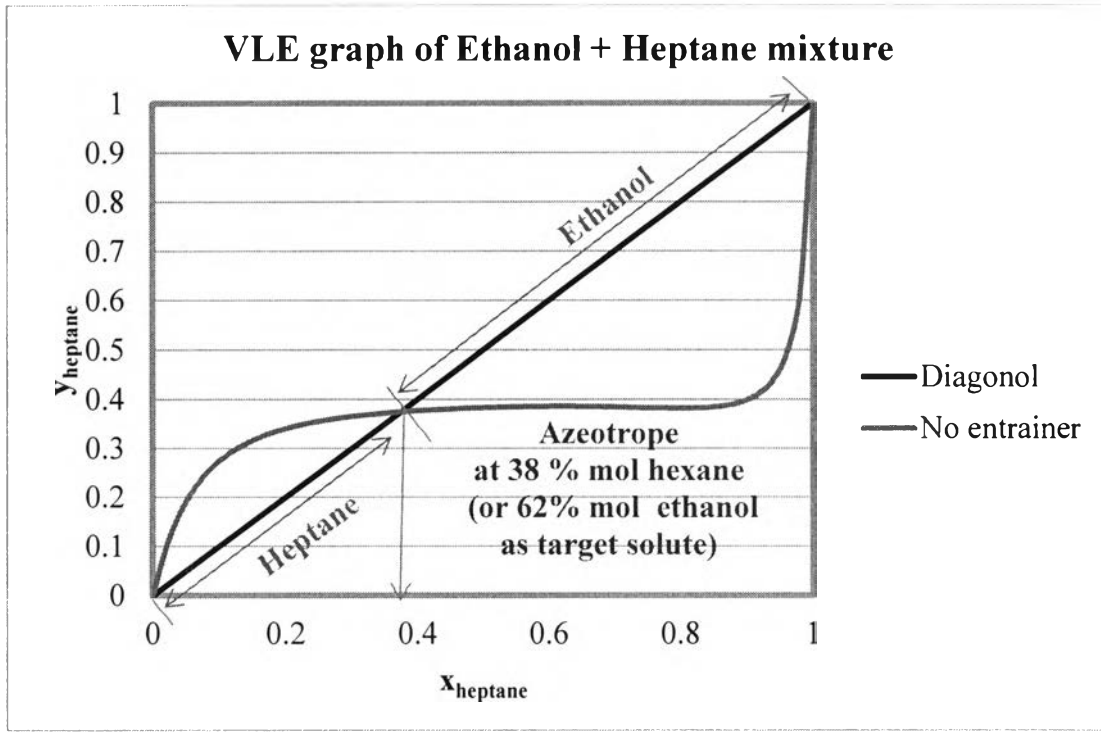

Figure I5 VLE graph of ethanol + heptane mixture.

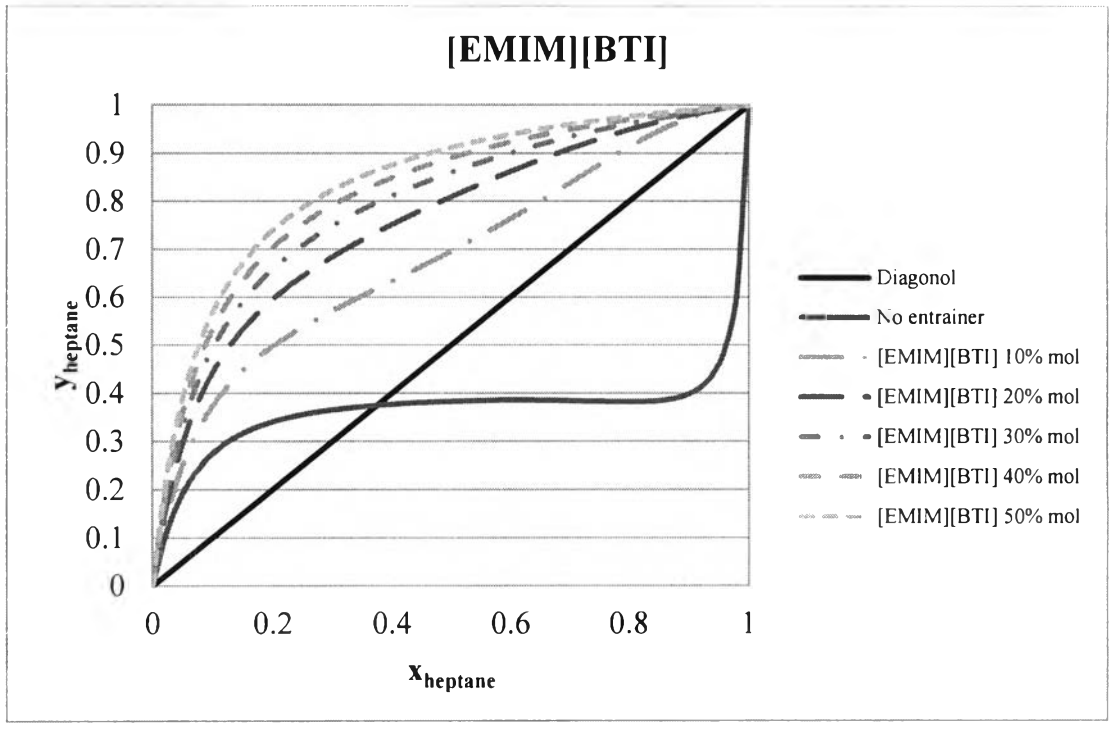

Figure I6 VLE graph of [EMIM][BTI] in ethanol + heptane mixture.

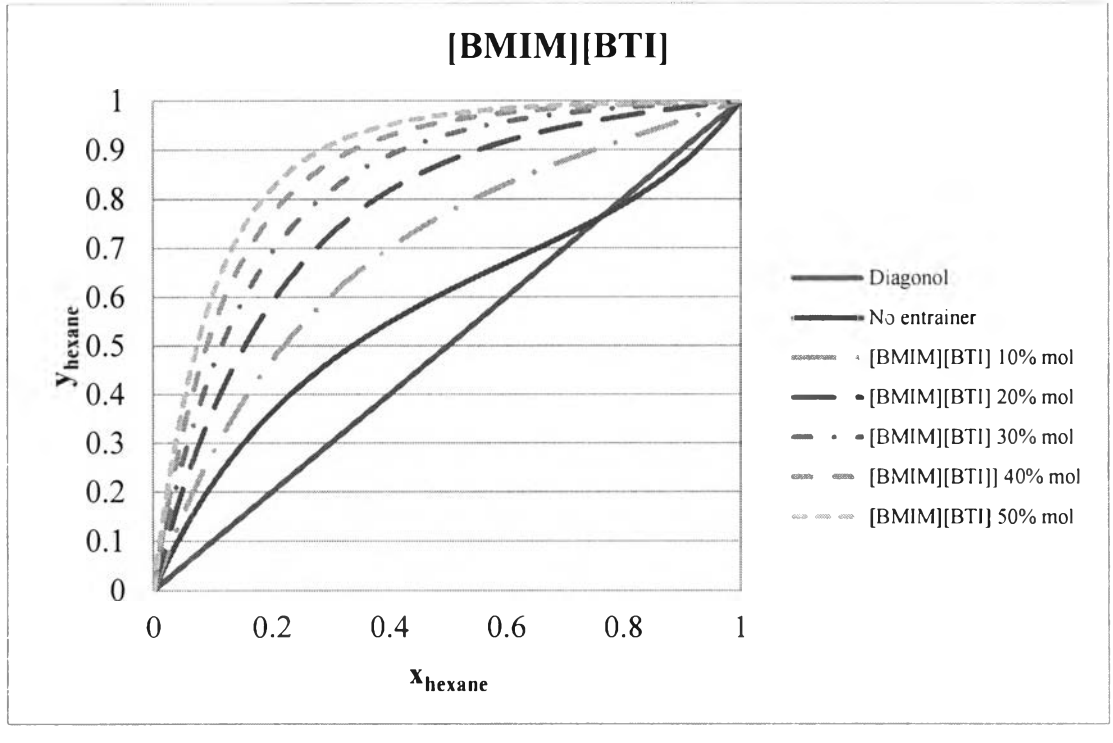

Figure I7 VLE graph of [BMIM][BTI] in ethanol + heptane mixture.

Appendix J Validation of Improved Screening Criteria in IL Pre-Selection Step

To validate the feasible IL candidates from the improved screening criteria in the IL pre-selection step, it showed a good agreement with other methodologies from several literatures of four case studies as listed in Table J1.

According to Hernández (2013), the methodology involved with a quantum calculation model by using COSMOtherm software. Two feasible IL candidates in water + ethanol mixture and six feasible IL candidates in toluene + MCH mixtures were reported. The liquid-liquid extraction experiment was demonstrated and used as the screening criteria in the method proposed by Meindersma *et al.* (2010). Three feasible IL candidates in benzene + hexane mixture have been reported. In Pereiro *et al.* (2012) literature, it has been reported that three, nine, and two feasible IL candidates were found in water + ethanol, benzene + hexane, and ethanol + hexane mixtures, respectively. Unfortunately, there were not enough the related literatures or researches in ethylbenzene (EB) + p-xylene (PX) to study in advance.

Table J1 Feasible IL candidates from other methodologies which are matched with the improved screening criteria

Case study	The feasible IL candidates from other methodologies which were matched with the improved screening criteria in IL pre-selection step		
	Hernández (2013)	**Meindersma *et al.* (2010)**	**Pereiro *et al.* (2012)**
	ILs	**ILs**	**ILs**
Water + Ethanol	[EMIM][DCA] and [MMIM][DMP]		[EMIM][EtSO4], [EMIM][DCA], and [MMIM][DMP]
Ethanol + Hexane	-		[HMIM][PF6] and [OMIM][BF4]
Benzene + Hexane		[E3S][BTI], [EMPYR][CF3SO3], and [EMIM][EtSO4]	[E3S][BTI], [EMIM][EtSO4], [OMIM][BTI], [HMIM][BTI], [BMPY][BTI], [BMIM][BTI], [EMIM][BTI], [MMIM][BTI], and [BMPYR][TCB]
Toluene + MCH	[HMPIP][BTI], [PeMPIP][BTI], [HMIM][TCB], [HMIM][BTI], [EMIM][TCB], and [EMIM][BTI]		-
EB + PX	-		-

To deeply validate in the technique of the improved screening criteria proposed in this work. It is emphasized to investigate the ILs that not passed the criteria and appeared outside of range or target window. These ILs must be confirmed that they are not suitable to be the feasible IL candidates.

Three scenarios are presented: (1) a very low capacity and selectivity or lower both minimum capacity and selectivity, i.e. [EMIM][BTI] in water + ethanol mixture, (2) a very high selectivity or higher than the maximum selectivity, i.e. [BMPY][TOS] in ethanol + hexane mixture, and (3) the influence of the Hildebrand solubility parameter.

1) A very low capacity and selectivity, i.e. [EMIM][BTI] in water + ethanol mixture

[EMIM][BTI] (Capacity = 0.29 and Selectivity = 0.59) highlighted by the violet dash square in the figure J1 is one of the ILs that not passed and showed very low capacity and selectivity or lower than both minimum capacity and selectivity in water + ethanol mixture. To check the separation capability for breaking azeotrope by VLE and compare it with others at 40% mole of each IL in Figure J2, [EMIM][BTI] cannot break the azeotrope. The VLE plot also shows that [EMIM][BTI] prefers to extract ethanol as compared to water. The vapor pressure and heat of vaporization of the two components show that water is higher in vapor pressure and lower in heat of vaporization than ethanol. It is obvious why the capacity and selectivity of [EMIM][BTI] in water are very low and not suitable for water + ethanol mixture. It is logically reasonable that [EMIM][BTI] turned out the best IL in ethanol + hexane mixture, where ethanol is the target solute.

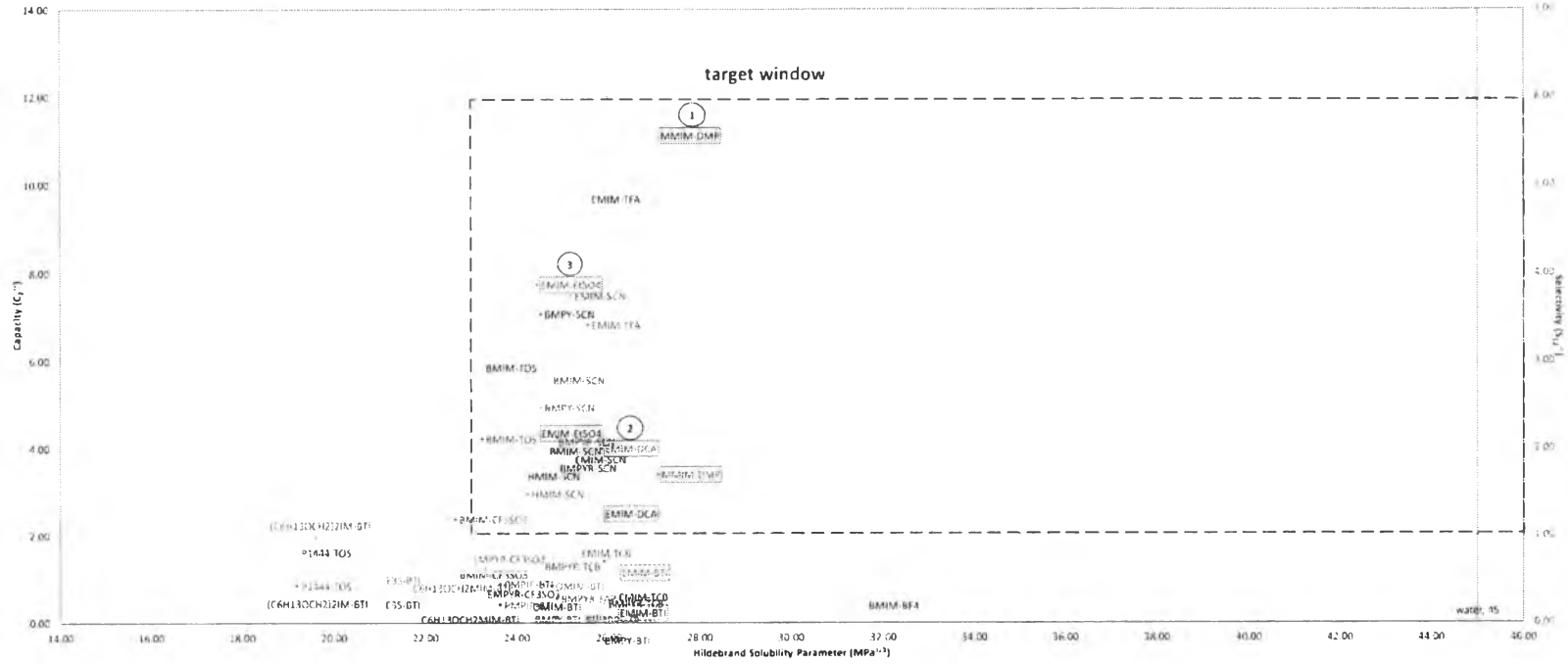

Figure J1 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the water + ethanol mixture. Water is the target solute.

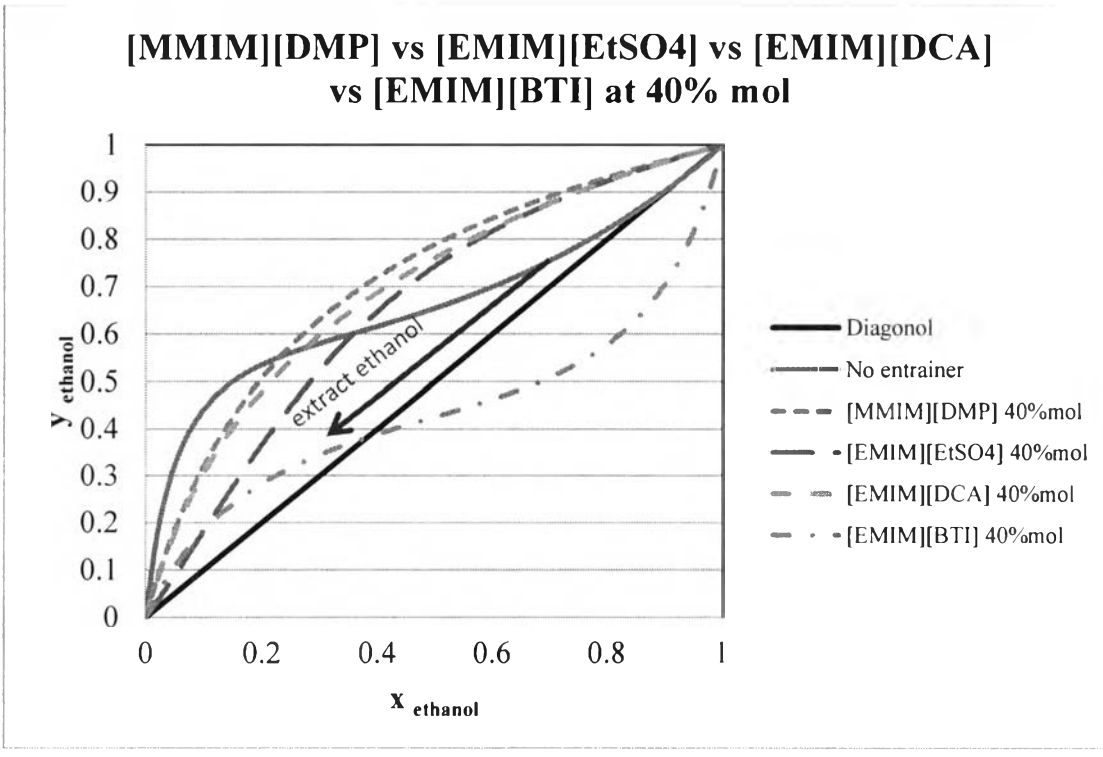

Figure J2 VLE comparison graph for separation capability of ILs in water + ethanol mixture.

2) A very high selectivity case, i.e. [BMPY][TOS] in ethanol + hexane mixture

[BMPY][TOS] (Capacity = 1.03, Selectivity = 49.15) in Figure J3 is one of the ILs that do not pass the screening criteria because of its very high selectivity or higher than the maximum selectivity but the capacity is still in the target window. To check the separation capability for breaking azeotrope by the VLE graph and compare it with other ILs at 30% mole of each IL in Figure J4, it showed the best separation capability as compared to the others. [BMPY][TOS] also exhibited that Hildebrand solubility parameter close to ethanol. Nevertheless, the comparison of simulation processes in Table J2 between [BMPY][TOS] process illustrated in Figure 5 and the best IL

([EMIM][EtSO4]) process is conversely turned out that [BMPY][TOS] needs higher energy requirement than the best IL. This phenomenon might be possible to occur owing to the difficulty of IL recovery process due to its high selectivity in the target solute as discussed in the work of Topphoff *et al.* (1999) and Hernández (2013). Hence, the feasible IL candidates should be avoided to select the very high capacity and selectivity. These are the reasons either why the improved screening criteria should limit the maximum capacity and selectivity. Since the default range could not be successful in the primary, the target window has been extended until finally to get the two feasible IL candidates, which have NRTL data to do further in the comparison stage.

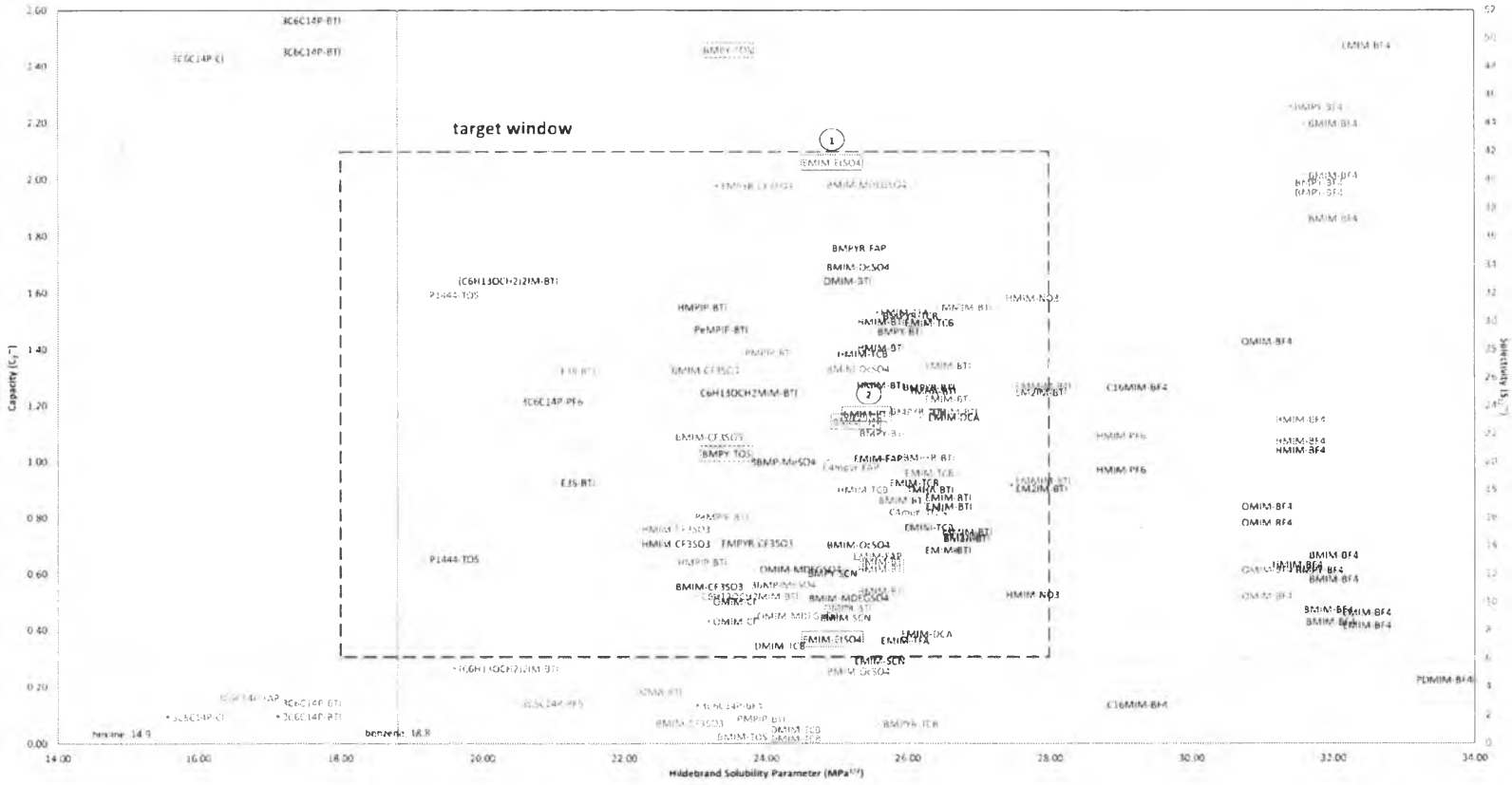

Figure J3 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^{∞}) of ILs (primary *y-axis*) and Selectivity (S_{12}^{∞}) of ILs (secondary *y-axis*) of the benzene + hexane mixture. Benzene is the target solute.

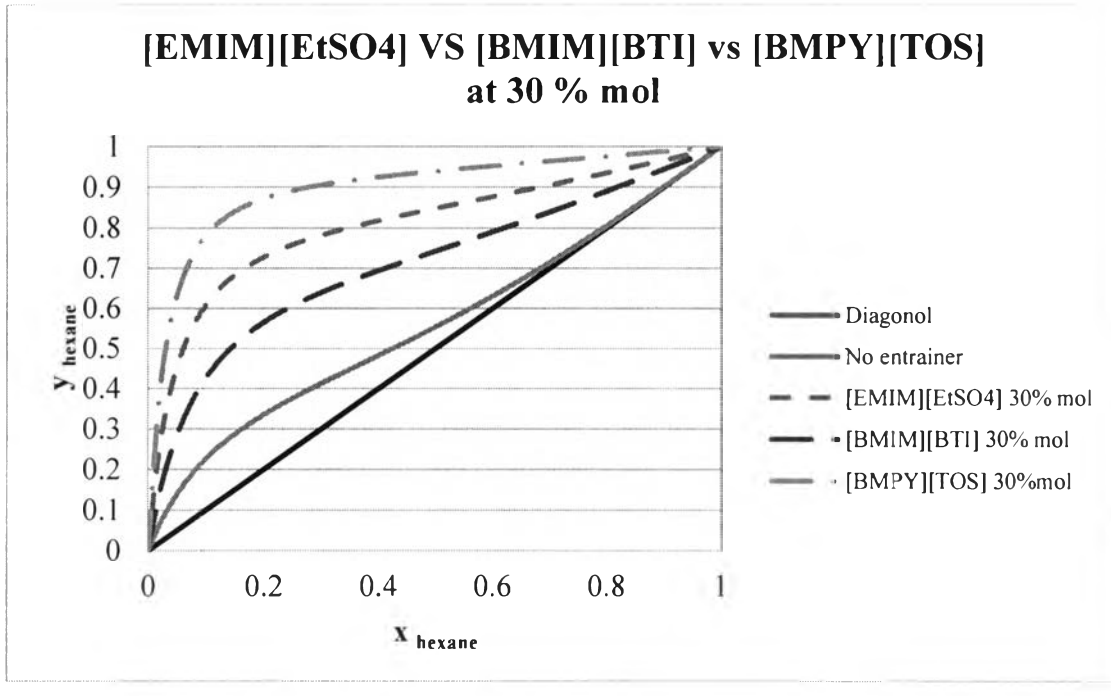

Figure J4 VLE comparison graph for separation capability of ILs in benzene + hexane mixture.

Table J2 Comparison between the solvent rate and energy requirement of both two ILs (e.g. [BMPY][TOS] and [EMIM][EtSO4]) processes

Topic \ **IL**		**[BMPY][TOS]**	**[EMIM][EtSO4]**
Solvent rate (kmol/hr)		200	400
Energy requirement (MW)	Q_{EDC}	3.1	3.4
	Q_{flash}	7.5	6.2
	Q_{E-R}	1.9	0.1
	Q_{E-F}	1.9	1.9
	Q_{E-D1}	0.7	0.7
	Q_{E-D2}	10.2	9.2
	Q_{E-D3}	1.9	1.9
	Q_{total}	27.2	23.4

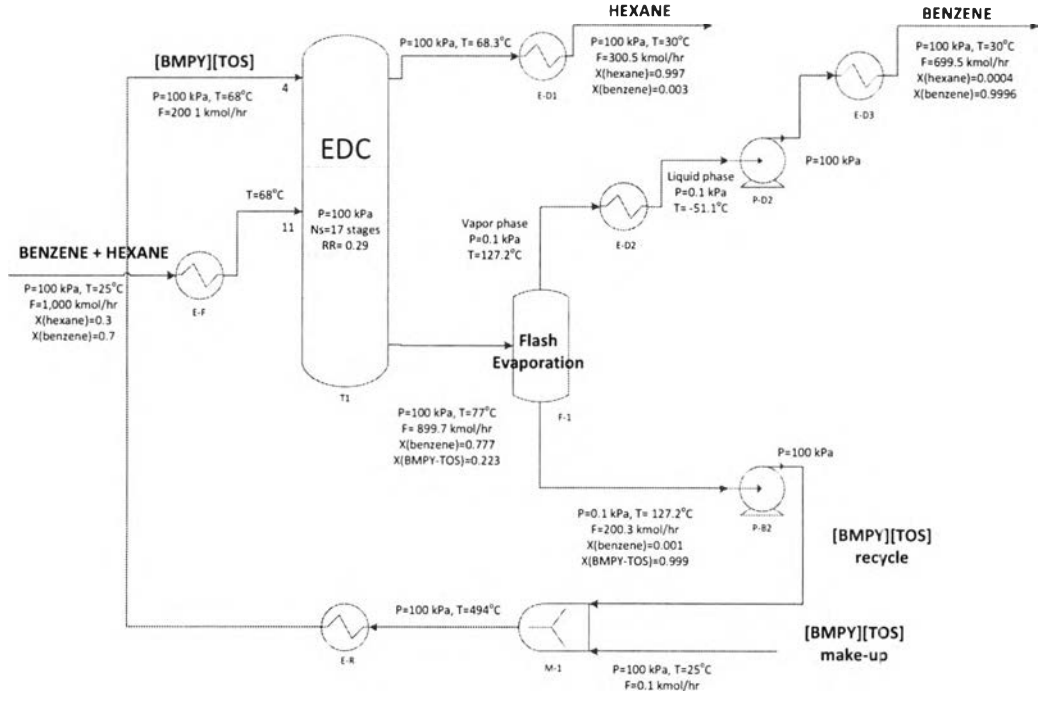

Figure J5 IL process flowsheet in benzene + hexane mixture using [EMPY][TOS].

3) The influence of the Hildebrand solubility parameter.

For the Hildebrand solubility parameter plotted in x-axis, the influence of target solute is evidenced by the ranking of feasible IL candidates from all results and showed a good corresponding with four case studies in Figures J1, J3, J6, and J7:

- From Figure J1 in water + ethanol mixture: [MMIM][DMP] is closer to water than [EMIM][DC A] and [EMIM][EtSO4], respectively
- From Figure J3 in benzene + hexane mixture: [EMIM][EtSO4] is closer to water than [BMIM][BTI]
- From Figure J6 in ethanol + hexane mixture: [EMIM][BTI] is closer to water than [BMIM][BTI]
- From Figure J7 in toluene + MCH mixture: [HMIM][TCB] is closer to water than [HMIM][BTI]

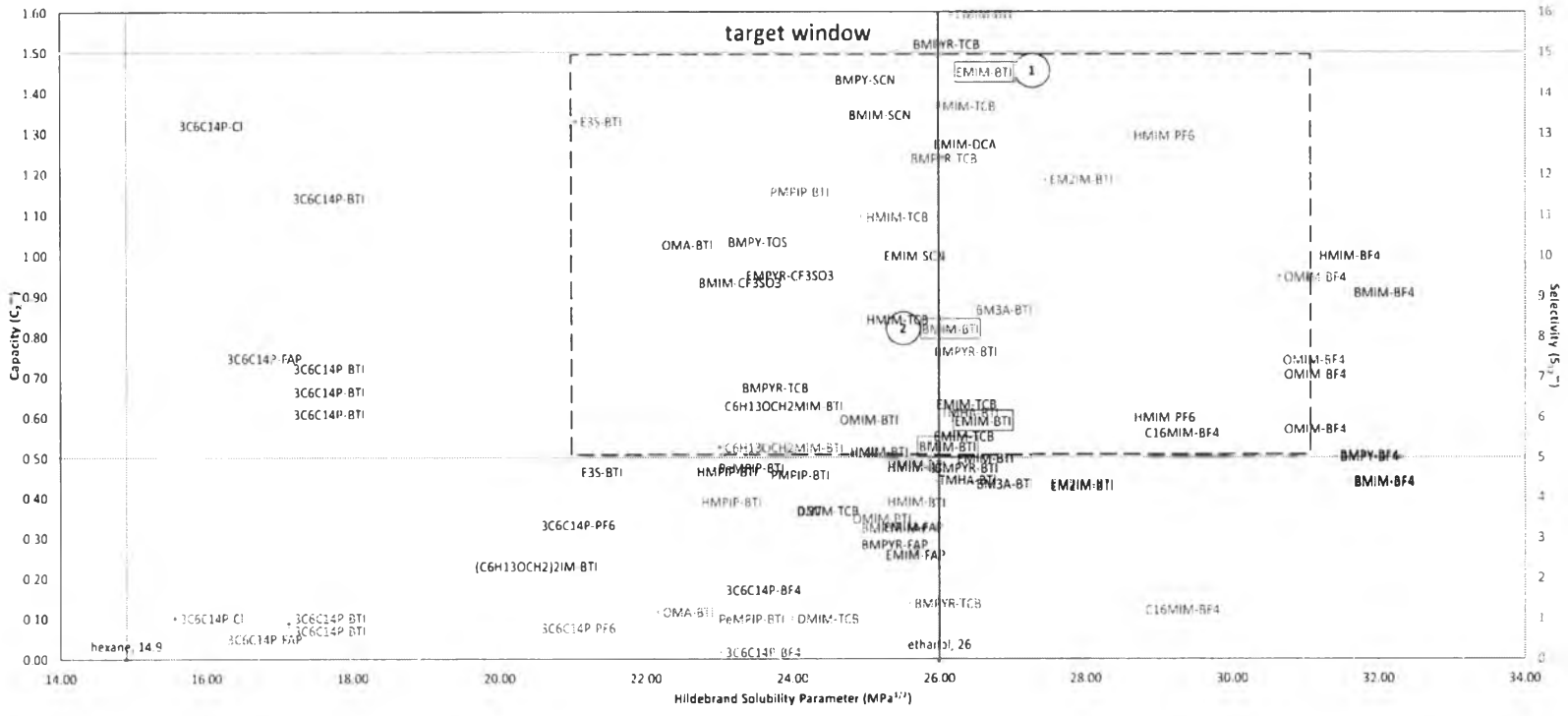

Figure J6 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the ethanol + hexane mixture. Ethanol is the target solute.

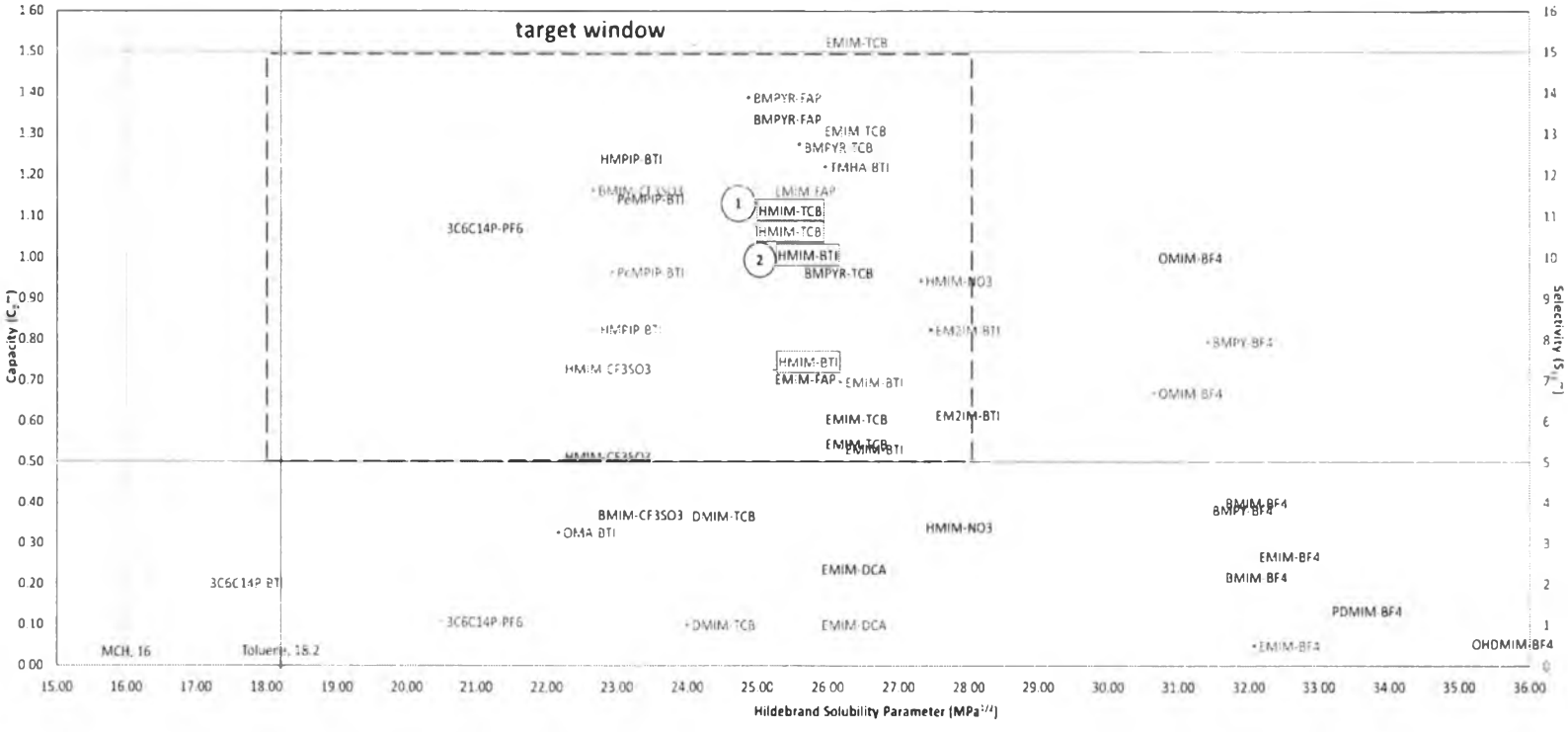

Figure J7 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^∞) of ILs (primary *y-axis*) and Selectivity (S_{12}^∞) of ILs (secondary *y-axis*) of the toluene + MCH mixture. Toluene is the target solute.

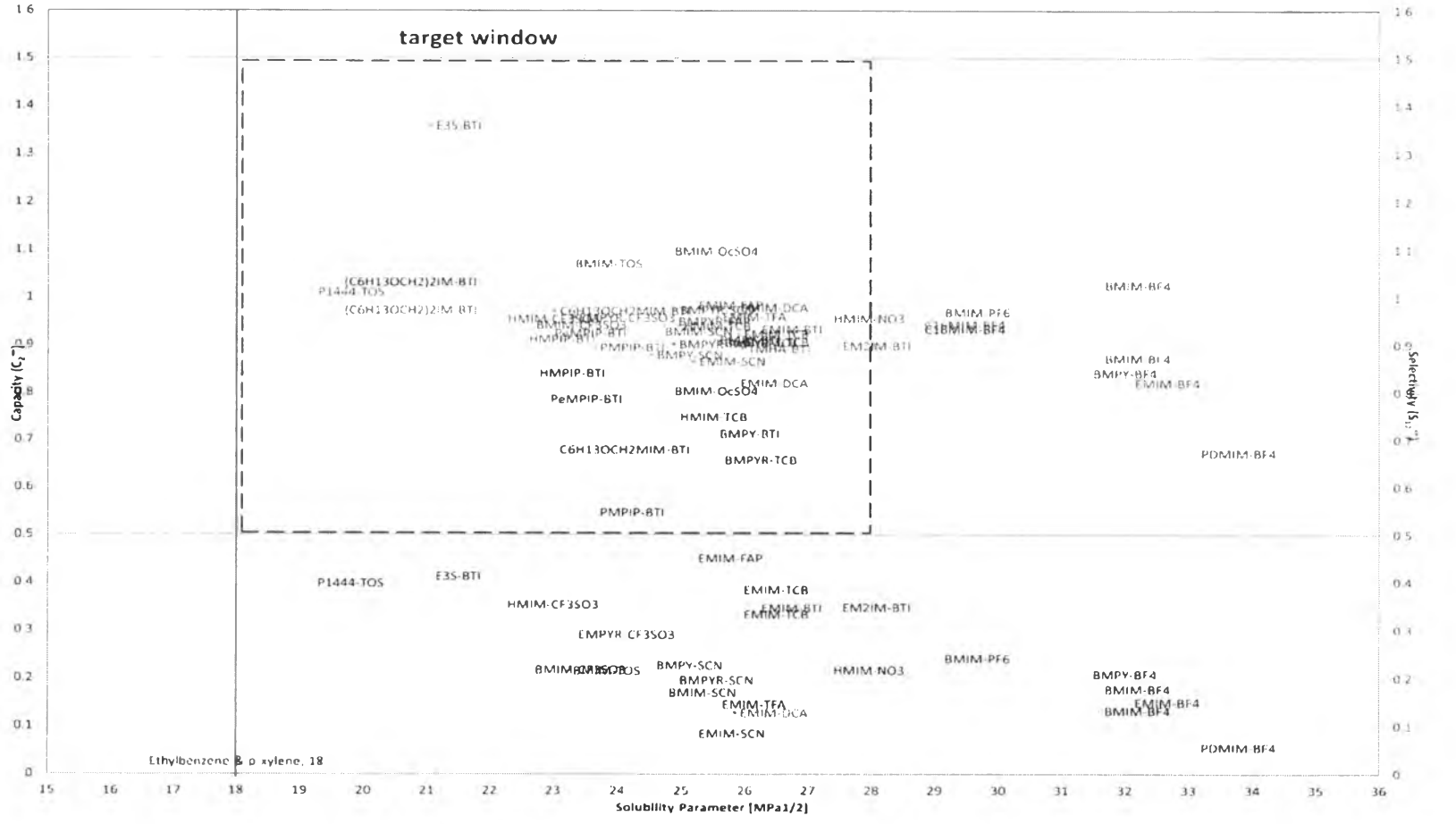

Figure J8 Hildebrand solubility parameters of ILs (*x-axis*) vs Capacity (C_2^{∞}) of ILs (primary *y-axis*) and Selectivity (S_{12}^{∞}) of ILs (secondary *y-axis*) of the EB + PX mixture. EB is the target solute.

To summarize, the suitable range is significantly considered for the improved screening criteria to generate the target window in screening graph. In this work, it needs to set the default range for the first guess of a user; however, the user can examine precisely about the target window from the first and second plots of screening graphs.
Due to the limitation of data in EB + PX mixture, there are no literatures about the researches of this mixture with ILs. Therefore, it is absolutely not able to prove it in this study. Beyond that, the NRTL data of several ILs in both cases of feasible IL candidates and the ILs not passed from the improved screening criteria are insufficient to validate in various scenarios. It is worth noting that the best ILs in this contribution was obtained from available 90 ILs from the literature database at the moment. Since IL data have been updating continuously, the IL database is suggested to be updated and re-run to seek for the updated best ILs of a particular azeotropic system when data become available.

Appendix K Comparison of Recovery Process between Using SRC and Flash Drum in Ethanol + Hexane Mixture

For comparison of recovery process between using SRC and Flash drum in ethanol + hexane mixture, all results are summarized in Table K1. The CS (Sulfolane) process and the best IL ([EMIM][BTI]) process of ethanol + hexane mixture in this contribution are the process number 1 and 8, respectively.

To begin with the process number 1 by suddenly changing the type of solvent entrainers from sulfolane to [EMIM][BTI], it became the process number 3 and could not run. Until decreasing the pressure of SRC at the deep vacuum pressure (0.1 kPa), it turned out to be the process number 4 as shown in Figure K1 and gave a lower energy requirement. If it re-increased the pressure of SRC to find the maximum value, it was found at 1 kPa as illustrated in the process number 5, which existed running the entire process. After that, it was adjusted the quantity of [EMIM][BTI] rate from 1,500 to 1,100 kmol/hr as following the process number 6, which was influenced to the lower energy requirement. Over again to decrease the pressure of SRC back at 0.1 kPa as the process number 7, it was similar to the best IL process in number 8 but used flash drum as recovery process instead of SRC and gave the lower energy requirement. On the other hand, if the pressure of SRC was adjusted at 0.1 kPa as the process number 2, it incredibly showed the very low energy requirement. However, the operation of recovery process at the deep vacuum pressure (0.1 kPa) should be concerned including investment and maintenance, especially, if it was existed the SRC. Therefore, the deep vacuum flash drum (0.1 kPa) is the alternative equipment which can be used instead of the deep vacuum SRC (0.1 kPa). According to (Meindersma *et al.* (2010), Hernández (2013), Lei *et al.* (2014a), Lei *et al.* (2014b)), they proposed the two potential technologies of recovery process for ILs from their works: (1) using only a flash drum and (2) using the combination of a flash drum and stripper with nitrogen or ethylbenzene (EB) except this technology is not supported in non-aqueous system.

In case of the product purity, the sulfolane process reached the maximum purity at 99.8% of hexane, 99.9% of ethanol and ~100% of solvent recycle but [EMIM][BTI] in the process number 9 by using flash drum as shown in Figure K2

could approach to almost 100% of all product purity. Moreover, it gave a lower energy requirement as compared to sulfolane in the process number 1. Beyond that, the demonstration of [EMIM][BTI] process by using SRC, the results showed the pressure of SRC operated at the 0.1 kPa in the process number 11 could be running. Nevertheless, the process number 11 operated at 1 kPa has found that the temperature of SRC is higher than the degradation temperature of [EMIM][BTI] (287°C) so the results cannot be used for comparison. To conclude, the separation capability of [EMIM][BTI] is better than sulfolane and can approach to almost 100% of all product purity whatever using SRC or flash drum as recovery process. For the operation of a deep vacuum flash drum, it should be seriously considered to use instead of a deep vacuum SRC.

Table K1 Summarized results from the comparison of recovery process between using SRC and flash drum in ethanol + hexane mixture

No.	Solvent entrainer	Solvent Rate (kmol/hr)	Recovery Process		Total Energy Requirement (MW)	Product Purity (%)			Remark
			type	Pressure (kPa)		Hexane	Ethanol	Solvent Recycle	
1	Sulfolane	1,500	SRC	75	57.3	99.8	99.9	~100	
2	Sulfolane	1,500	SRC	0.1	21.55	99.8	99.9	~100	
3	[EMIM][BTI]	1,500	SRC	75	-	99.8	99.9	~100	Not run
4	[EMIM][BTI]	1,500	SRC	0.1	28.5	99.8	99.9	~100	
5	[EMIM][BTI]	1,500	SRC	1	31.4	99.8	99.9	~100	
6	[EMIM][BTI]	1,100	SRC	1	30.1	99.8	99.9	~100	
7	[EMIM][BTI]	1,100	SRC	0.1	28.3	99.8	99.9	~100	
8	[EMIM][BTI]	1,100	flash	0.1	32.2	99.8	99.9	~100	
9	[EMIM][BTI]	1,100	flash	0.1	39.9	~100	~100	~100	
10	[EMIM][BTI]	1,100	SRC	0.1	37.2	~100	~100	~100	
11	[EMIM][BTI]	1,100	SRC	1	40.2	~100	~100	~100	$T_{SRC} > T_{degradation}$

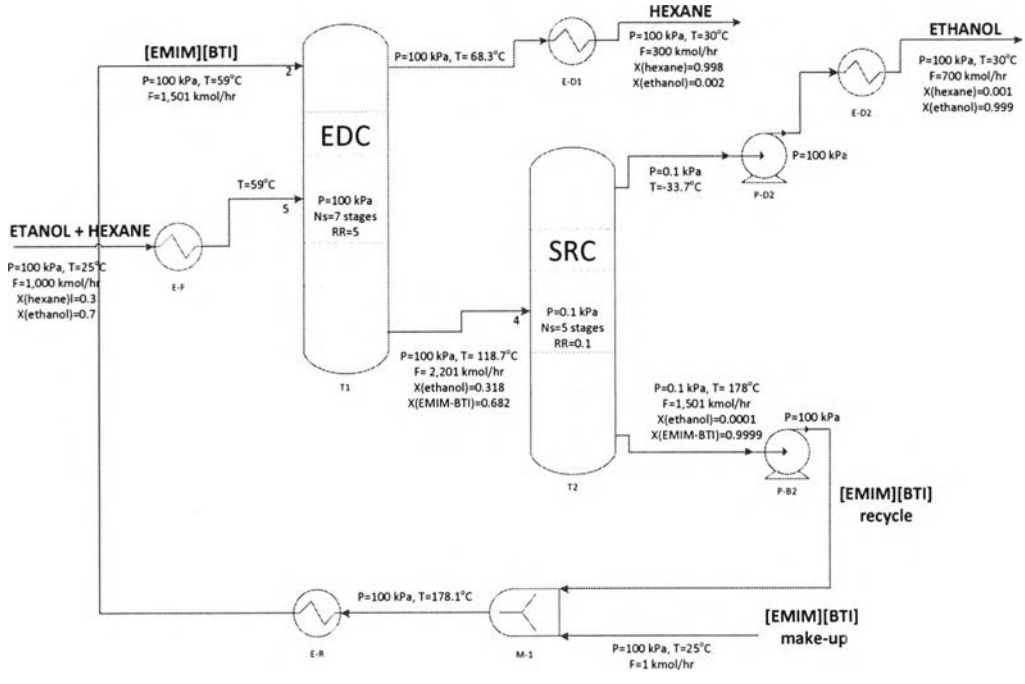

Figure K1 IL process flowsheet in ethanol + hexane mixture using [EMIM][BTI] (No.4).

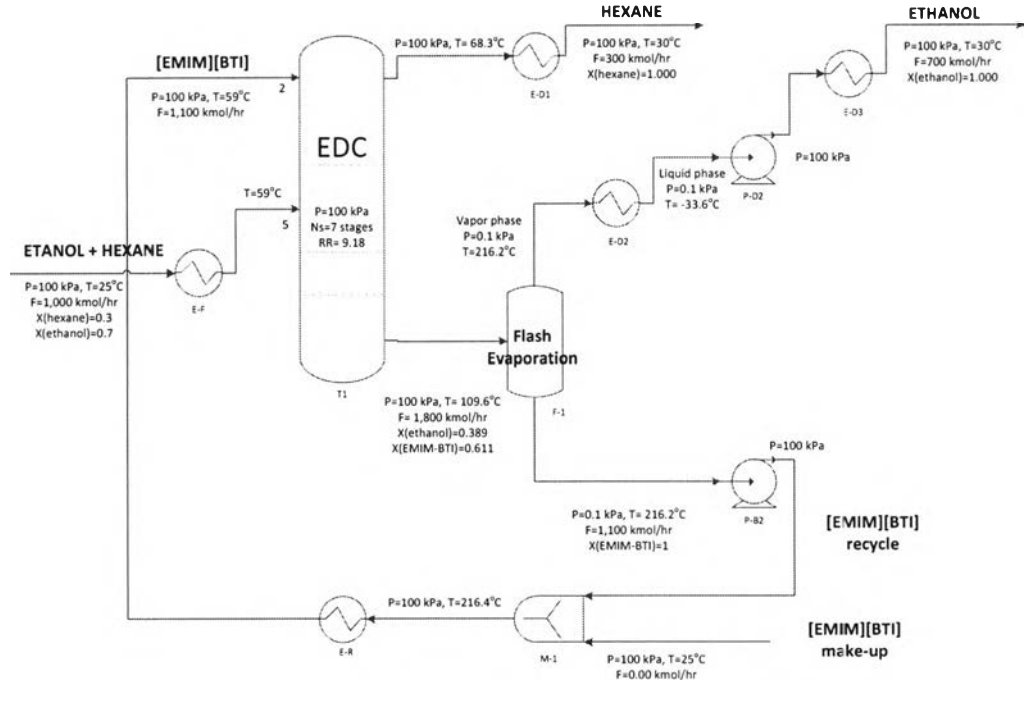

Figure K2 IL process flowsheet in ethanol + hexane mixture using [EMIM][BTI] (No.9).

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Proceedings:

1. Peng-noo, W.; Suriyapraphadilok, U.; and Gani, R. (2015, April 21) Design and Use of Ionic Liquids in Separation Processes for Azeotropic Mixtures. Proceedings of the 6th Research Symposium on Petrochemical and Materials Technology and the 21th PPC Symposium on Petroleum, Petrochemicals, and Polymers, Bangkok, Thailand.
2. Peng-noo, W,; Kulajanpeng, K.; Suriyapraphadilok, U.; and Gani, R. (2015, May 31 - June 4) Design of Separation Processes with Ionic Liquids. Proceeding of the 12th International Symposium on Process Systems Engineering and 25th European Symposium on Computer Aided Process Engineering, Lyngby, Denmark.