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APPENDICES

Appendix A: Critical Properties Estimation

Appendix A1: The modified Lyndersen-Joback-Reid group contribution method

The modified Lyndersen-Joback-Reid group contribution method is used to estimated the properties of ionic liquid [emim][Ac]. Those properties including the normal boiling temperature (T_b), the critical properties (T_c, P_c, and V_c), and the acentric factors (ω).

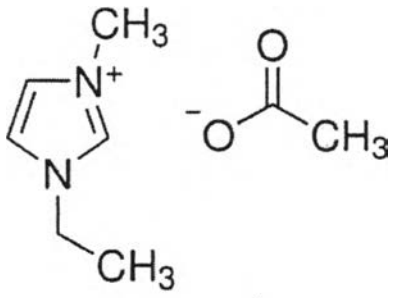
Mw = 170.21

A_M = 0.5703

B_M = 1.0121

C_M = 0.2573

E_M = 6.75



$$T_b = 198.2 + \sum n\Delta T_{bM} \qquad P_c = \frac{M}{[C_M + \sum n\Delta P_M]^2}$$

$$T_c = \frac{T_b}{A_M + B_M \sum n\Delta T_M - (\sum n\Delta T_M)^2} \qquad V_c = E_M + \sum n\Delta V_M$$

$$\omega = \frac{(T_b - 43)(T_c - 43)}{(T_c - T_b)(0.7T_c - 43)} \log\left[\frac{P_c}{P_b}\right] - \frac{(T_c - 43)}{(T_c - T_b)} \log\left[\frac{P_c}{P_b}\right] + \log\left[\frac{P_c}{P_b}\right] - 1$$

Table A1 The normal boiling temperature, critical properties, and acentric factor of [emim][Ac]

Groups	Number	ΔTbm	ΔTm	ΔPm	ΔVm	n*ΔTbm	n*ΔTm	n*ΔPm	n*ΔVm
Cation									
-CH3 (nonring)	2	23.58	0.0275	0.3031	66.81	47.16	0.055	0.6062	133.62
-CH2- (nonring)	1	22.88	0.0159	0.2165	57.11	22.88	0.0159	0.2165	57.11
=CH- (ring)	3	26.73	0.0114	0.1693	42.55	80.19	0.0342	0.5079	127.65
-N= (ring)	2	57.55	-0.0011	0.0559	42.15	115.1	-0.0022	0.1118	84.3
Anion									
-COO-(nonring)	1	81.1	0.0377	0.4139	84.76	81.1	0.0377	0.4139	84.76
-CH3 (nonring)	1	23.58	0.0275	0.3031	66.81	23.58	0.0275	0.3031	66.81
SUM						370.01	0.1681	2.1594	554.25

Note: T_b = 568.21 K; T_c = 797.8501 K; P_c = 29.14336 bar; V_c = 561 cm^3/mol, ω = 0.54919501

To ensure that the selected group contributions for calculating the properties of ionic liquid [emim][Ac] are correct, I previously calculated the properties of ionic liquid [emim][TFA] that has the molecular structure resemble to [emim][Ac] and compared with the values reported in the literature. The calculation values are equal to the reported value. (Critical Properties, Normal Boiling Temperatures, and Acentric Factors of Fifty Ionic Liquid,; J. O. Valderrama, and P. A. Robles).

Appendix A2: Verification of the modified Lyndersen-Joback-Reid group contribution method

In order to verify the modified Lyndersen-Joback-Reid method, the liquid density of ionic liquid [emim][Ac] from the literature is determined as a consistency test for the estimated properties using a generalized correlation based on the equation of Spencer and Danner(Spencer and Danner, 1972), which requires the normal boiling temperature, the molecular weight, and the critical properties.

$$\rho_L = \frac{MP_c}{RT_c}\left[\frac{0.3445P_cV_c^{1.0135}}{RT_c}\right]^{\Omega} \qquad \Omega = -\left[\frac{1+(1-T_R)^{2/7}}{1+(1-T_{bR})^{2/7}}\right]$$

Table A2 The calculated density of [emim][Ac] and comparison with the experimental values at a range of temperature from 383.15 K to 363.15 K

T (K)	TR	Ω	ρexp (g/cm3)	ρcal (g/cm3)	%Δρcal
283.15	0.354891	-1.10684	1.0472	1.156163	10.40518
288.15	0.361158	-1.1054	1.0429	1.152037	10.46478
293.15	0.367425	-1.10394	1.0385	1.147897	10.53415
298.15	0.373692	-1.10248	1.0342	1.143743	10.59203
303.15	0.379959	-1.101	1.0299	1.139574	10.64898

308.15	0.386225	-1.09951	1.0256	1.13539	10.70495
313.15	0.392492	-1.09802	1.0213	1.131191	10.75992
318.15	0.398759	-1.09651	1.017	1.126977	10.81385
323.15	0.405026	-1.09499	1.0127	1.122747	10.86668
328.15	0.411293	-1.09346	1.0084	1.118501	10.9184
333.15	0.41756	-1.09191	1.0041	1.114239	10.96895
338.15	0.423826	-1.09036	0.9998	1.109961	11.01828
343.15	0.430093	-1.08879	0.9958	1.105666	11.0329
348.15	0.43636	-1.08721	0.9915	1.101353	11.07952
353.15	0.442627	-1.08562	0.9872	1.097024	11.12478
358.15	0.448894	-1.08401	0.9828	1.092677	11.17996
363.15	0.455161	-1.0824	0.9785	1.088311	11.22242
				AAD (%)	0.214398

The estimated density of ionic liquid [emim][Ac] are within acceptable range of errors. The AAD for [emim][Ac] is 0.214 % Density ref. Thermophysical Properties of Five Acetate-Based Ionic Liquids; Hugo F. D. Almeida, Helena Passos, José A. Lopes-da-Silva, Ana M. Fernandes, Mara G. Freire,,and João A. P. Coutinho.

Appendix B: Temperature-dependent Correlation Parameters for [emim][Ac] Properties

Appendix B1: Heat of formation, Gibbs Energy of Formation and Heat of Vaporization (at normal boiling point)

Joback group contribution method is used to estimate heat of formation, Gibbs energy of formation and heat of vaporization (at normal boiling point) of ionic liquid [emim][Ac].

Table B1 Heat of formation, Gibbs energy of formation and heat of vaporization (at normal boiling point) of ionic liquid [emim][Ac]

			Chemical Caloric Properties		Enthalpy of Phase Transition	Chemical Caloric Properties		Enthalpy of Phase Transition
	Groups	Number	Hform	Gform	Hvap	n*Hform	n*Gform	n*Hvap
Cation	-CH3 (nonring)	2	-76.45	-43.96	2.373	-152.9	-87.92	4.746
	-CH2- (nonring)	1	-20.64	8.42	2.226	-20.64	8.42	2.226
	=CH- (ring)	3	2.09	11.3	2.544	6.27	33.9	7.632
	-N= (ring)	2	55.52	79.93	6.528	111.04	159.86	13.056
Anion	-COO-(nonring)	1	-337.92	-301.95	9.633	-337.92	-301.95	9.633
	-CH3 (nonring)	1	-76.45	-43.96	2.373	-76.45	-43.96	2.373
	SUM					-470.6	-231.65	39.666

Note: Hform = -402.31 kJ/mol, Gform = -177.77 kJ/mol; Hvap = 54.966 kJ/mol.

Appendix B2: Specific Heat Capacity

The Joback method is used to estimate specific heat capacity of ionic liquid [emim][Ac] due to this property isn't available in the literature. The Joback method uses a four parameter polynomial to describe the temperature dependency of the ideal gas heat capacity. These parameters are valid from 273 K to approx. 1000 K.

$$C_P = \sum a_i - 37.93 + \left[\sum b_i + 0.210\right] T + \left[\sum c_i - 3.91 \cdot 10^{-4}\right] T^2 + \left[\sum d_i + 2.06 \cdot 10^{-7}\right] T^3$$

Table B2.1 Group contribution of specific heat capacity of ionic liquid [emim][Ac]

Groups	Number	a	b	c	d	an	bn	cn	dn
Cation									
-CH3 (nonring)	2	1.95E+01	-8.08E-03	1.53E-04	-9.67E-08	3.90E+01	-1.62E-02	3.06E-04	-1.93E-07
-CH2- (non-ring)	1	-9.09E-01	9.50E-02	-5.44E-05	1.19E-08	-9.09E-01	9.50E-02	-5.44E-05	1.19E-08
=CH- (ring)	3	-2.14	5.74E-02	-1.64E-06	-1.59E-08	-6.42E+00	1.72E-01	-4.92E-06	-4.77E-08
-N= (ring)	2	8.83	-3.84E-03	4.35E-05	-2.60E-08	1.77E+01	-7.68E-03	8.70E-05	-5.20E-08
Anion									
-COO- (nonring)	1	2.45E+01	4.02E-02	4.02E-05	-4.52E-08	2.45E+01	4.02E-02	4.02E-05	-4.52E-08

-CH3 (nonring)	1	19.5	-0.00808	0.000153	-9.7E-08	1.95E+01	-8.08E-03	1.53E-04	-9.67E-08
SUM						9.33E+01	2.75E-01	5.27E-04	-4.23E-07

Table B2.2 Estimated specific heat capacity of ionic liquid [emim][Ac] at a range of temperature from 273 K to 473 K.

T (K)	J/mol.K	T (K)	J/mol.K	T (K)	J/mol.K	T (K)	J/mol.K
273	193.6468	323	219.0714	373	244.1235	423	268.6403
278	196.2014	328	221.596	378	246.6019	428	271.0562
283	198.7537	333	224.1168	383	249.0749	433	273.4651
288	201.3036	338	226.6335	388	251.5421	438	275.8666
293	203.8509	343	229.146	393	254.0035	443	278.2606
298	206.3955	348	231.6541	398	256.459	448	280.6471
303	208.9371	353	234.1577	403	258.9082	453	283.0257
308	211.4757	358	236.6566	408	261.3511	458	285.3964
313	214.011	363	239.1507	413	263.7875	463	287.7589
318	216.543	368	241.6397	418	266.2173	468	290.1132

Note: Correlation coefficient $R^2 = 0.999868$ (Estimation).

Specific Heat Capacity Regression

Aspen ideal gas heat capacity polynomial (CPIG) is used for regression of specific heat capacity of ionic liquid [emim][Ac].

$$C_p^{*ig} = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 + C_{6i}T^5 \text{for} \; C_{7i} \leq T \leq C_{8i}$$

$$C_p^{*ig} = C_{9i} + C_{10i}T^{C} \quad \text{for} \; T < C_{7i}$$

Table B2.3 Temperature-dependent correlation parameter of ideal gas heat capacity of ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (K; J/kmol.K)
CPIG/1	C1i	67576.78
CPIG/2	C2i	588.599
CPIG/3	C3i	0.102842
CPIG/4	C4i	0
CPIG/5	C5i	0
CPIG/6	C6i	0
CPIG/7	C7i	0
CPIG/8	C8i	1000
CPIG/9	C9i	0
CPIG/10	C10i	0

Table B2.4 Comparison of specific heat capacity of ionic liquid [emim][Ac] between Estimated and Regression

T (K)	J/mol.K		T (K)	J/mol.K		T (K)	J/mol.K		T (K)	J/mol.K	
	Estimation	Regression		Estimation	Regression		Estimation	Regression		Estimation	Regression
273	193.6468	-	323	219.0714	-	373	244.1235	-	423	268.6403	-
278	196.2014	-	328	221.596	-	378	246.6019	-	428	271.0562	-
283	198.7537	-	333	224.1168	-	383	249.0749	-	433	273.4651	-
288	201.3036	-	338	226.6335	-	388	251.5421	-	438	275.8666	-
293	203.8509	248.8652	343	229.146	-	393	254.0035	-	443	278.2606	-
298	206.3955	252.1121	348	231.6541	-	398	256.459	-	448	280.6471	-
303	208.9371	255.3641	353	234.1577	-	403	258.9082	-	453	283.0257	-
308	211.4757	258.6213	358	236.6566	-	408	261.3511	-	458	285.3964	-
313	214.011	261.8836	363	239.1507	-	413	263.7875	-	463	287.7589	-
318	216.543	265.1511	368	241.6397	-	418	266.2173	-	468	290.1132	-

Note: Correlation coefficient $R^2 = 0.999999$ (regression); AAD % between estimation and regression = 0.0391.

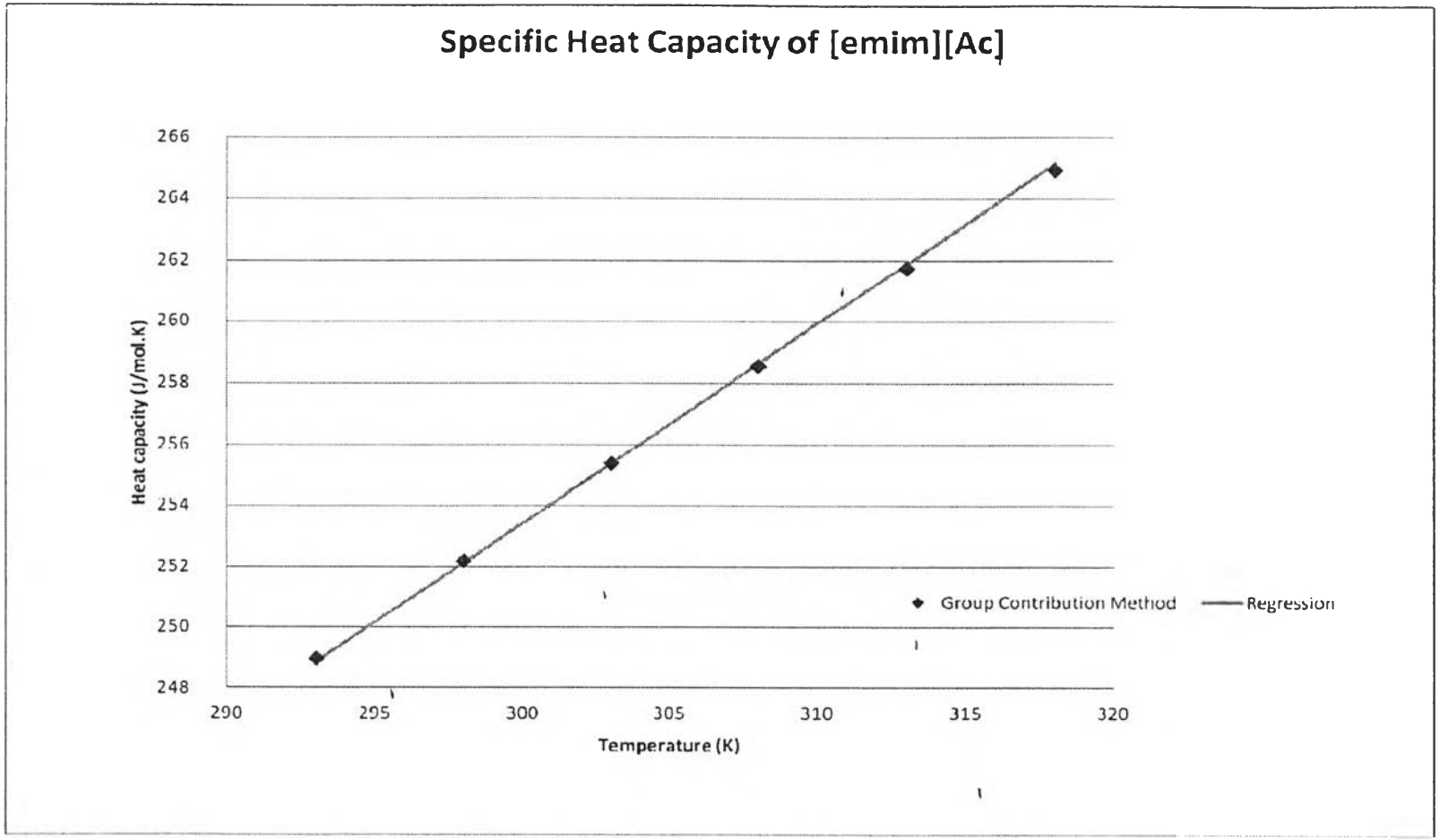


Figure B2 Comparison of specific heat capacity between estimation and regression of ionic liquid [emim][Ac].

Appendix B3: Liquid Vapor Pressure

Rudkin (1961), considered water as reference fluid and use Antoine equation to relate the vapor pressure of any fluid with the temperature T. Rudkin used a value C = 43 (with T in Kelvin), value corresponding to water, the reference fluid. The equation is:

$$\log P^S = A - \frac{B}{T - 43}$$

$A = \text{Log}(P_c)*(T_c\text{-}43)/(T_c\text{-}T_b)$

$B = \text{Log}(P_c)*(T_c\text{-}43)*(T_b\text{-}43)/(T_c\text{-}T_b)$

Ref: Critical Properties, Normal Boiling Temperatures, and Acentric Factors of Fifty Ionic Liquids; J. O. Valderrama, and P. A. Robles, Critical Properties and Vapor Pressure of Twenty Imidazolium based Ionic Liquids used in Extraction Bioprocesses; . J. O. Valderrama and Wilson W. Sanga.

Table B3.1 Estimated vapor pressure of ionic liquid [emim][Ac] at a range of temperature from 273.15 K to 523.15 K.

T (K)	P (Pa)	T (K)	P (Pa)
273.15	6.73248E-07	413.15	0.009623285
283.15	1.93035E-06	423.15	0.014554907
293.15	5.0877E-06	433.15	0.021551843
303.15	1.24466E-05	443.15	0.031292397
313.15	2.8498E-05	453.15	0.044616543
323.15	6.15028E-05	463.15	0.062548886
333.15	0.000125877	473.15	0.086321954
343.15	0.000245626	483.15	0.117399418
353.15	0.00045907	493.15	0.157498813
363.15	0.000825118	503.15	0.208613359
373.15	0.00143129	513.15	0.273032506
383.15	0.002403667	523.15	0.353360857
393.15	0.003918871		
403.15	0.006218116		

Note: Correlation coefficient $R^2 = 0.58679$ (Estimation).

Liquid Vapor Pressure Regression

Extended Antoine equation - Aspen (PLXANT) is used for regression of vapor pressure of ionic liquid [emim][Ac].

$$\ln p_i^{sat} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i} T + C_{5i} \ln T + C_{6i}\ T^{C_{7i}} \text{ for } C_{8i} \le T \le C_{9i}$$

Table B3.2 Temperature-dependent correlation parameter of ideal gas heat capacity of ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (K; Pa)
PLXANT/1	C1i	5.549195
PLXANT/2	C2i	-5756.1
PLXANT/3	C3i	-43.715
PLXANT/4	C4i	-2.78E-04
PLXANT/5	C5i	0.518242
PLXANT/6	C6i	4.738097
PLXANT/7	C7i	-0.11424
PLXANT/8	C8i	0
PLXANT/9	C9i	1000

Table B3.3 Comparison of specific heat capacity of ionic liquid [emim][Ac] between Estimated and Regression

T (K)	Pa		T (K)	Pa		T (K)	Pa	
	Estimation	Regression		Estimation	Regression		Estimation	Regression
273.15	6.73248E-07	6.7319E-07	373.15	0.00143129	0.001431239	473.15	0.086321954	0.086324971
283.15	1.93035E-06	1.93036E-06	383.15	0.002403667	0.002403581	483.15	0.117399418	0.117403019
293.15	5.0877E-06	5.08792E-06	393.15	0.003918871	0.003918748	493.15	0.157498813	0.157501995
303.15	1.24466E-05	1.24472E-05	403.15	0.006218116	0.006217969	503.15	0.208613359	0.208613914
313.15	2.8498E-05	2.84993E-05	413.15	0.009623285	0.009623155	513.15	0.273032506	0.273026292
323.15	6.15028E-05	6.15046E-05	423.15	0.014554907	0.014554877	523.15	0.353360857	0.353340783
333.15	0.000125877	0.000125879	433.15	0.021551843	0.021552049			
343.15	0.000245626	0.000245624	443.15	0.031292397	0.031293029			
353.15	0.00045907	0.00045906	453.15	0.044616543	0.044617823			
363.15	0.000825118	0.000825092	463.15	0.062548886	0.06255101			

Note: Correlation coefficient $R^2 = 0.5868$ (regression); AAD % between estimation and regression = 0.00283.

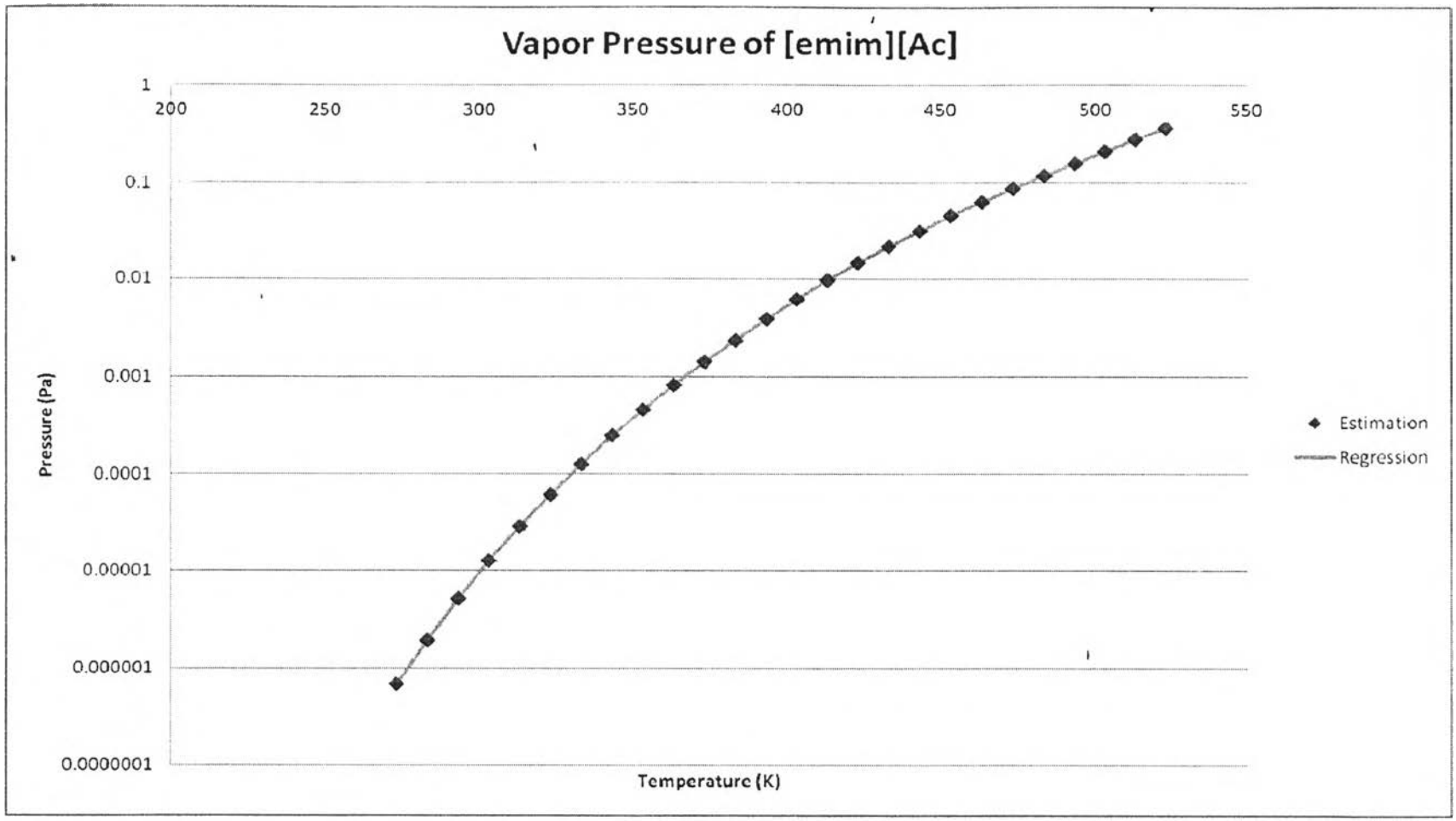


Figure B3 Comparison of vapor pressure between estimation and regression of ionic liquid [emim][Ac].

Appendix B4: Density

Ref: Thermophysical Properties of Five Acetate-Based Ionic Liquids; Hugo F. D. Almeida,[1]Helena Passos, José A. Lopes-da-Silva, Ana M. Fernandes, Mara G. Freire, and João A. P. Coutinho.

Density Regression

DIPPR equation 105 - Aspen (DNLDIP) is used for regression of liquid density of ionic liquid [emim][Ac].

$$\rho_i = C_{1i} / C_{2i}^{[1+(1-T/C_{3i})^{C_{4i}}]} \quad \text{for } C_{6i} \le T \le C_{7i}$$

Table B4.1 Temperature-dependent correlation parameter of liquid density of ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (K; kmol/cum)
DNLDIP/1	C1i	0.37252
DNLDIP/2	C2i	0.220678
DNLDIP/3	C3i	1110.037
DNLDIP/4	C4i	0.528581
DNLDIP/5	C5i	0
DNLDIP/6	C6i	0
DNLDIP/7	C7i	1000

Table B4.2 Density of ionic liquid [emim][Ac] at a range of temperature from 283.15 K to 363.15 K.

T (K)	Kg/cum		T (K)	Kg/cum	
	Experiment	Regression		Experiment	Regression
283.15	1047.177	1.047177	328.15	1008.442	1.008442
288.15	1042.852	1.042852	333.15	1004.165	1.004165
293.15	1038.531	1.038531	338.15	999.8931	0.999893
298.15	1034.217	1.034217	343.15	995.6264	0.995626
303.15	1029.908	1.029908	348.15	991.3648	0.991365
308.15	1025.604	1.025604	353.15	987.1084	0.987108
313.15	1021.305	1.021305	358.15	982.857	0.982857
318.15	1017.012	1.017012	363.15	978.6107	0.978611
323.15	1012.725	1.012725			

Note: Correlation coefficient $R^2 = 0.999992$ (regression); AAD % between experiment and regression = 0.00554.

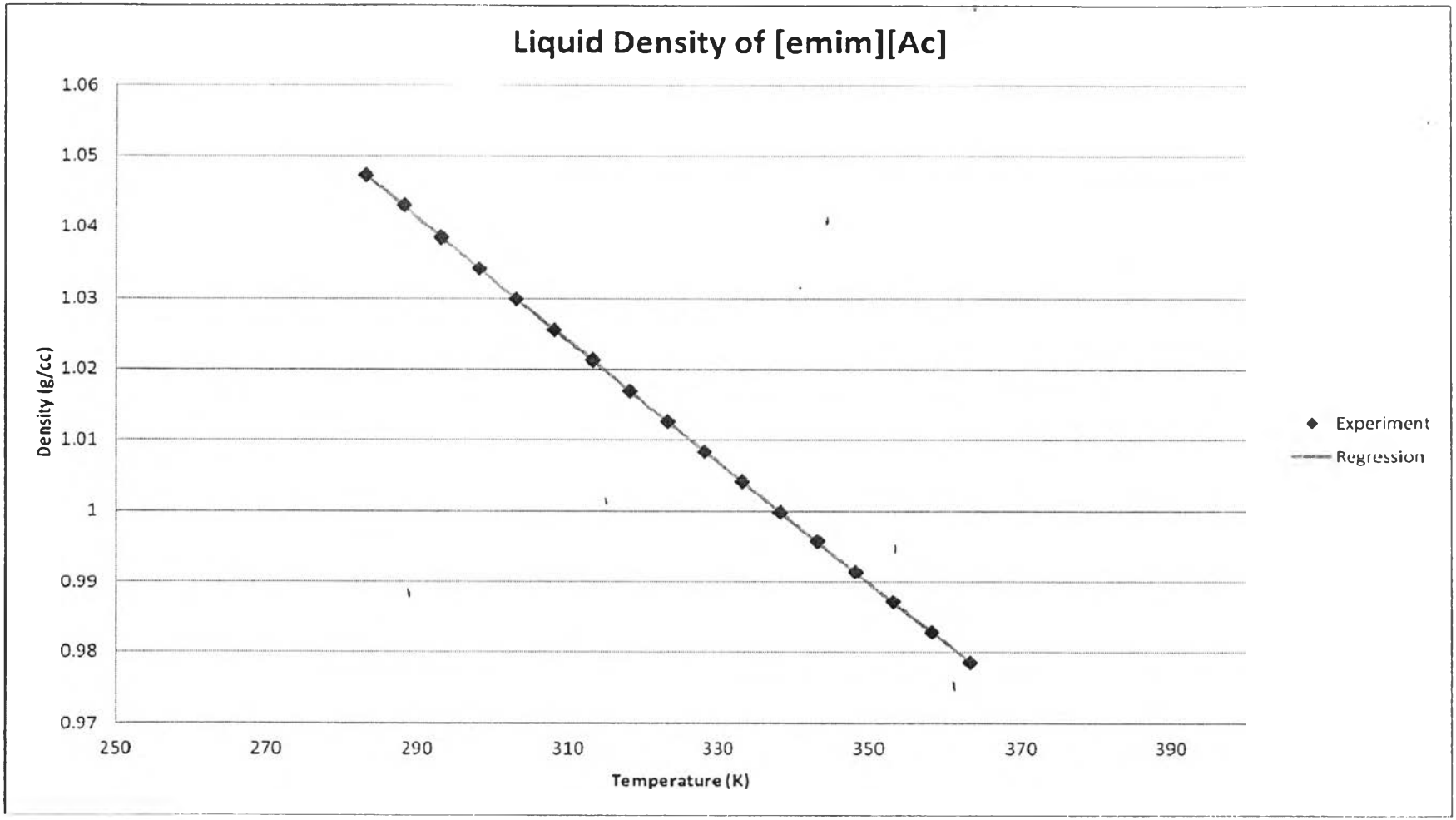


Figure B4 Comparison of liquid density between the experiment and regression of ionic liquid [emim][Ac].

Appendix B5: Viscosity

Ref: : Thermophysical Properties of Five Acetate-Based Ionic Liquids; Hugo F. D. Almeida, Helena Passos, José A. Lopes-da-Silva, Ana M. Fernandes, Mara G. Freire, and João A. P. Coutinho.

Viscosity Regression

DIPPR liquid viscosity equation - Aspen (MULDIP) is used for regression of liquid viscosity of ionic liquid [emim][Ac].

$$\ln \eta_i^{*,l} = C_{1i} + C_{2i}/T + C_{3i} \ln T + C_{4i} T^{C} \quad \text{for} \quad C_{6i} \le T \le C_{7i}$$

Table B5.1 Temperature-dependent correlation parameter of liquid viscosity of ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (K; N-sec/sqm)
MULDIP/1	C1i	-321.912
MULDIP/2	C2i	20301.95
MULDIP/3	C3i	46.42677
MULDIP/4	C4i	-7.05354
MULDIP/5	C5i	-0.06058
MULDIP/6	C6i	0
MULDIP/7	C7i	1000

Table B5.2 Viscosity of ionic liquid [emim][Ac] at a range of temperature from 283.15 K to 363.15 K.

T (K)	mPa.s (cp)		T (K)	mPa.s (cp)	
	Experiment	Regression		Experiment	Regression
283.15	1037	994.9578	328.15	52.8	52.58859
288.15	659	649.7145	333.15	42.7	42.12255
293.15	429	436.4739	338.15	34.7	34.31546
298.15	297	301.1559	343.15	28.7	28.40731
303.15	210	213.0847	348.15	24	23.87659
308.15	152	154.3896	353.15	20.8	20.35992
313.15	112	114.3953	358.15	17.5	17.60036
318.15	86.1	86.57284	363.15	15.1	15.41375
323.15	66.8	66.83953			

Note: Correlation coefficient $R^2 = 0.633963$ (regression); AAD % between experiment and regression = 1.3869.

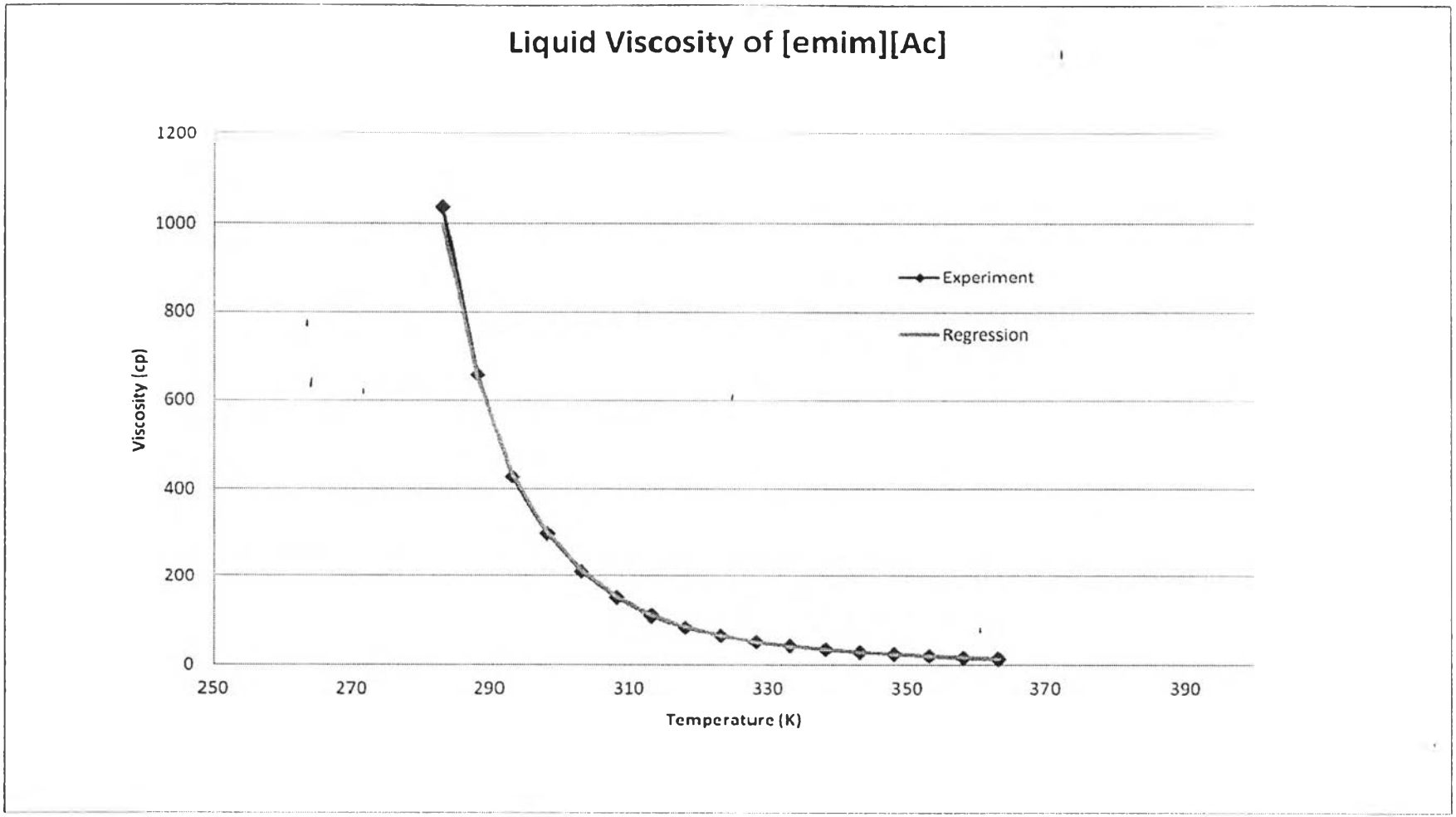


Figure B5 Comparison of liquid viscosity between the experiment and regression of ionic liquid [emim][Ac].

Appendix B6: Surface Tension

Ref: : (Thermophysical Properties of Five Acetate-Based Ionic Liquids; Hugo F. D. Almeida, Helena Passos, José A. Lopes-da-Silva, Ana M. Fernandes, Mara G. Freire, and João A. P. Coutinho.

Surface Tension Regression

DIPPR surface tension equation - Aspen (SIGDIP) is used for regression of surface tension of ionic liquid [emim][Ac].

$$\sigma_i^{*,1} = C_{1i} \cdot 1 - T_{ri}^{(C_{2i} + C_{3i} T_{ri} + C_{4i} T_{ri})} \quad \text{for} \quad C_{6i} \le T \le C_{7i}$$

Where:

T_{ri} = T / T_{ci}

Table B6.1 Temperature-dependent correlation parameter of surface tension of ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (K; N/m)
SIGDIP/1	C1i	0.027268
SIGDIP/2	C2i	-2.89365
SIGDIP/3	C3i	5.889673
SIGDIP/4	C4i	0

SIGDIP/5	C5i	0
SIGDIP/6	C6i	0
SIGDIP/7	C7i	1000

Table B6.2 Surface tension of ionic liquid [emim][Ac] at a range of temperature from 298.1 K to 344.2 K.

T (K)	mPa.s (cp)	
	Experiment	Regression
298.1	0.0378	0.037711
307.8	0.0367	0.036915
318.5	0.0361	0.035949
328.3	0.035	0.034986
339.9	0.0337	0.033757
344.2	0.0333	0.033278

Note: Correlation coefficient $R^2 = 0.992376$ (regression); AAD % between experiment and regression = 0.252292.

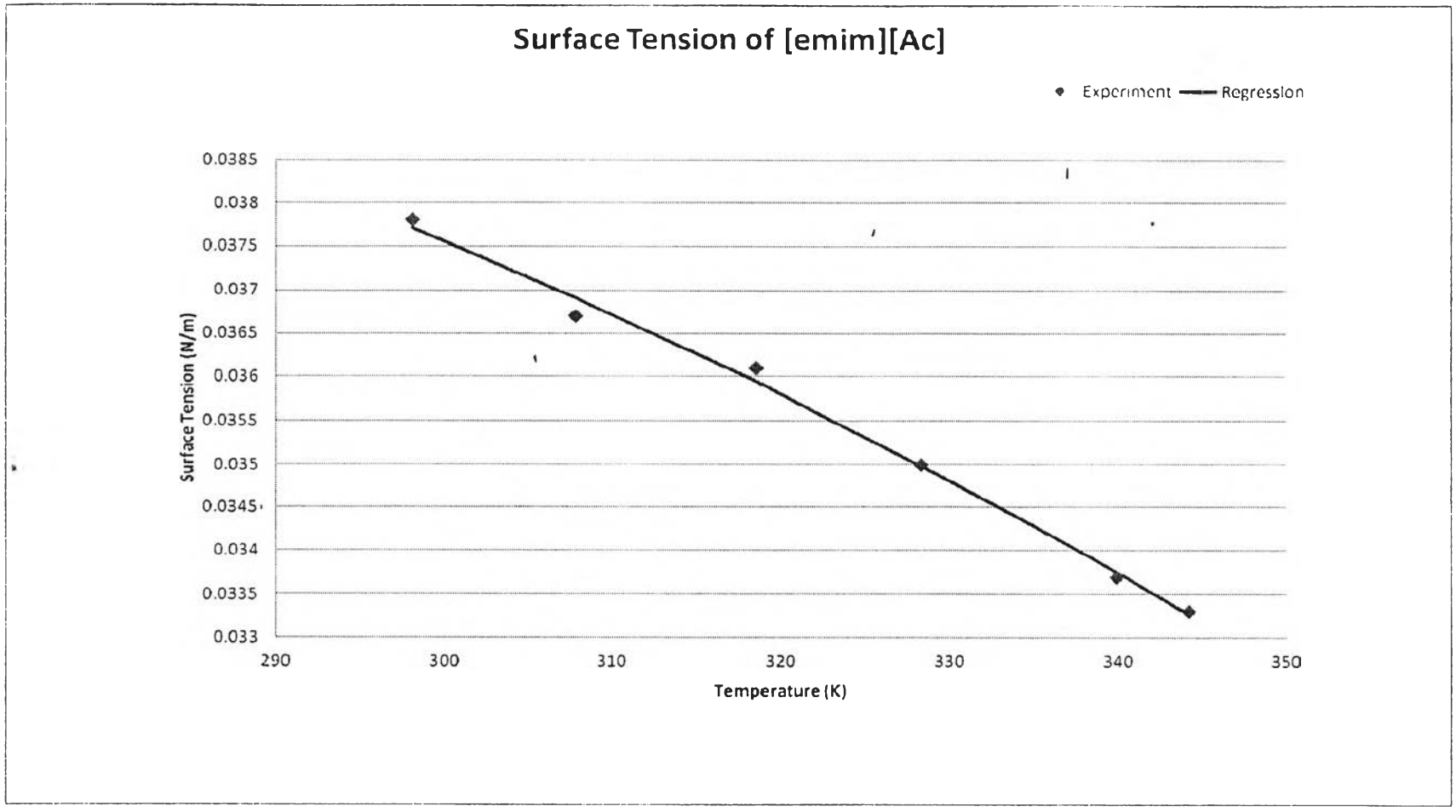


Figure B6 Comparison of surface tension between the experiment and regression of ionic liquid [emim][Ac].

Appendix C: Binary Interaction Parameters

Appendix C1: NRTL (Non-Random Two-Liquid)

The NRTL model- Aspen is used to calculate liquid activity coefficient of the binary system ([emim][Ac] + H2O). Theses binary interaction parameters are determined from data regression of the experimental VLE data for the system water + [emim][Ac] reported by Romich., et al (2012)

Ref: (Thermodynamic Properties of Binary Mixtures of Water and Room-Temperature Ionic Liquids: Vapor Pressures, Heat Capacities, Densities, and Viscosities of Water + 1-Ethyl-3-methylimidazolium Acetate and Water + Diethylmethylammonium Methane Sulfonate; Christiane Römich, Nina C. Merkel, Alessandro Valbonesi, Karlheinz Schaber, Sven Sauer, and Thomas J. S. Schubert.

General Equation

The general equation for $\ln(\gamma_i)$ for species i in a mixture of n components is:

$$\ln\gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right)$$

Where:

$$G_{ij} = \exp(-\alpha_{ij}\tau_{ij})$$

$$\tau_{ij} = a_{ij} + {}^{b_{ij}}/_{T} + e_{ij}\ln T + f_{ij}T$$

$$\alpha_{ij} = c_{ij} + d_{ij}(T - 273.15K)$$

Table C1.1 Binary interaction parameters (NRTL) of the binary system for water and ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (SI-Unit/ K)		Temperature (K)	$(g_{12}-g_{22})/R$	$(g_{21}-g_{11})/R$	α
NRTL/1	Aij	80		293.15	33452	-651.391	0.338354
NRTL/1	Aji	9.789126		303.15	34252	-553.5	0.338354
NRTL/2	Bij	10000		313.15	35052	-455.608	0.338354
NRTL/2	Bji	-3521.07		323.15	35852	-357.717	0.338354
NRTL/3	Cij	0.338354		333.15	36652	-259.826	0.338354
NRTL/4	Dij	0		343.15	37452	-161.935	0.338354
NRTL/5	Eij	0		353.15	38252	-64.0434	0.338354
NRTL/5	Eji	0		293.15	33452	-651.391	0.338354
NRTL/6	Fij	0					
NRTL/6	Fij	0					

Note: i=H_2O, J=[emim][Ac].

Note: $(g_{12}-g_{21})/R = [80 \times T(K)] + 10000$.

$(g_{21}-g_{12})/R = [9.789126 \times T(K)] - 3521.02$.

Table C1.2 Mole-fraction of water in binary mixture at a constant temperature 293.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
293.15	1.399994	1.437054	0.687	0.685665	-0.19428
293.15	3.599994	3.647154	0.745	0.736317	-1.16554
293.15	5.409999	5.454773	0.782	0.77092	-1.41694
293.15	7.819999	7.861823	0.818	0.806005	-1.46634
293.15	11.32	11.37188	0.855	0.843764	-1.31414
293.15	13.95	14.06442	0.886	0.876334	-1.09097
293.15	19.3	19.67812	0.933	0.927526	-0.58669
293.15	21.05	21.7142	0.957	0.953784	-0.33601
293.15	23.18	23.18595	1	1	0
				AAD (%)	0.499528

Table C1.3 Mole-fraction of water in binary mixture at a constant temperature 303.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
303.15	1.83	1.900698	0.612	0.613801	0.294281
303.15	3.049999	3.143644	0.655	0.653251	-0.26698
303.15	3.899999	4.00513	0.686	0.682204	-0.55335
303.15	8.219998	8.35135	0.745	0.737627	-0.98961
303.15	10.92	11.05929	0.782	0.773573	-1.07763
303.15	14.75	14.8991	0.818	0.809448	-1.04545
303.15	19.86	20.03551	0.855	0.847337	-0.89621
303.15	24.94	25.16822	0.885	0.878728	-0.7087
303.15	36.32	36.70818	0.933	0.929709	-0.35272
303.15	40.86	41.44449	0.957	0.955076	-0.20104
303.15	44.43	44.37213	1	1	0
				AAD (%)	0.383405

Table C1.4 Mole-fraction of water in binary mixture at a constant temperature 313.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
313.15	1.449995	1.532291	0.495	0.491625	-0.68186
313.15	2.709998	2.838861	0.553	0.549569	-0.62049
313.15	4.699997	4.88428	0.612	0.609088	-0.47583
313.15	8.669998	8.923388	0.655	0.650657	-0.66307
313.15	8.710002	8.970189	0.686	0.68115	-0.70695
313.15	14.85	15.17642	0.745	0.738905	-0.81807
313.15	18.89	19.25245	0.782	0.775633	-0.81426
313.15	25.44	25.83639	0.817	0.811	-0.73441
313.15	37.12	37.51012	0.855	0.850143	-0.56805
313.15	47.1	47.46804	0.885	0.881217	-0.42747
313.15	64.35	64.68505	0.933	0.930994	-0.21505
313.15	71.78001	72.15929	0.956	0.954768	-0.12885
313.15	77.86001	77.72191	1	1	0
				AAD (%)	0.213706

Table C1.5 Mole-fraction of water in binary mixture at a constant temperature 323.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
323.15	3.519994	3.722045	0.494	0.482776	-2.27211
323.15	5.329999	5.607396	0.553	0.541354	-2.106
323.15	8.189999	8.566639	0.612	0.606126	-0.95987
323.15	12.77	13.26739	0.654	0.648479	-0.84422
323.15	15.73	16.296	0.686	0.68062	-0.78423
323.15	25.05	25.77513	0.745	0.739889	-0.686
323.15	34.27	35.09078	0.781	0.776339	-0.59681
323.15	47.32	48.19139	0.817	0.813065	-0.4816
323.15	63.57	64.40459	0.854	0.850938	-0.35854
323.15	79.82998	80.51966	0.884	0.881683	-0.26215
323.15	105.59	105.9514	0.932	0.930751	-0.13402
323.15	116.02	116.2916	0.956	0.955225	-0.08108
323.15	126.69	126.5689	1	1	0
				AAD (%)	0.505685

Table C1.6 Mole-fraction of water in binary mixture at a constant temperature 333.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
333.15	6.449997	6.855167	0.494	0.476107	-3.62215
333.15	9.549997	10.10469	0.553	0.533929	-3.44861
333.15	14.71	15.47751	0.611	0.602281	-1.427
333.15	22.05	23.05894	0.654	0.647174	-1.04379
333.15	26.41	27.55476	0.686	0.68012	-0.8572
333.15	45.75	47.28352	0.744	0.739773	-0.56812
333.15	59.26	60.97274	0.781	0.777592	-0.43636
333.15	78.14001	79.94629	0.816	0.813376	-0.32162
333.15	103.64	105.3418	0.853	0.851115	-0.22094
333.15	127.52	128.9232	0.883	0.881618	-0.15657
333.15	166.52	167.1422	0.931	0.930257	-0.07986
333.15	182.77	183.0435	0.955	0.954528	-0.04948
333.15	199.28	199.2944	1	1	0
				AAD (%)	0.888916

Table C1.7 Mole-fraction of water in binary mixture at a constant temperature 343.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
343.15	10.9	11.66103	0.494	0.469747	-4.90951
343.15	16.11	17.16182	0.553	0.526985	-4.70436
343.15	23.24	24.65773	0.611	0.599622	-1.86223
343.15	37.34	39.31036	0.653	0.645021	-1.22188
343.15	47.01	49.31467	0.685	0.678795	-0.90588
343.15	75.57998	78.58024	0.743	0.739345	-0.4919
343.15	94.61999	97.94678	0.78	0.777395	-0.33397
343.15	122.92	126.4299	0.815	0.813236	-0.2164
343.15	161.62	164.94	0.852	0.850883	-0.13114
343.15	197.12	199.9037	0.882	0.881239	-0.08632
343.15	255.91	257.2226	0.93	0.929609	-0.04201
343.15	283.28	283.7417	0.954	0.953749	-0.02632
343.15	305.97	306.2785	1	1	0
				AAD (%)	1.246699

Table C1.8 Mole-fraction of water in binary mixture at a constant temperature 353.15 K

Temperature (K) (constant)	Pressure (mbar)		Mole fraction of water		AAD (%)
	Experiment	Regression	Experiment	Regression	
353.15	17.8	19.18268	0.494	0.463739	-6.12575
353.15	25.06	26.92083	0.552	0.519227	-5.93708
353.15	38.59	41.25021	0.611	0.597377	-2.22962
353.15	63.95	67.736	0.653	0.644265	-1.33763
353.15	76.86999	81.19231	0.684	0.677456	-0.95674
353.15	117.52	123.0458	0.742	0.738656	-0.4507
353.15	147	153.1048	0.778	0.775901	-0.26978
353.15	189.97	196.3973	0.814	0.81281	-0.14615
353.15	245.64	251.764	0.851	0.850391	-0.07157
353.15	298.54	303.7389	0.881	0.880661	-0.03846
353.15	386.79	389.4066	0.929	0.928864	-0.01469
353.15	429.49	430.4836	0.952	0.951913	-0.00918
353.15	463.22	463.8397	1	1	0
				AAD (%)	1.574436

Table C1.9 Average absolute deviation (AAD%) between experimental and estimated value of mole fraction by the NRTL for the [emim][Ac] + H_2O system

	Temperature (K)							Average
	293.15	303.15	313.15	323.15	333.15	343.15	353.15	AAD (%)
AAD (%)	0.499528	0.383405	0.213706	0.505685	0.888916	1.246699	1.574436	0.758911

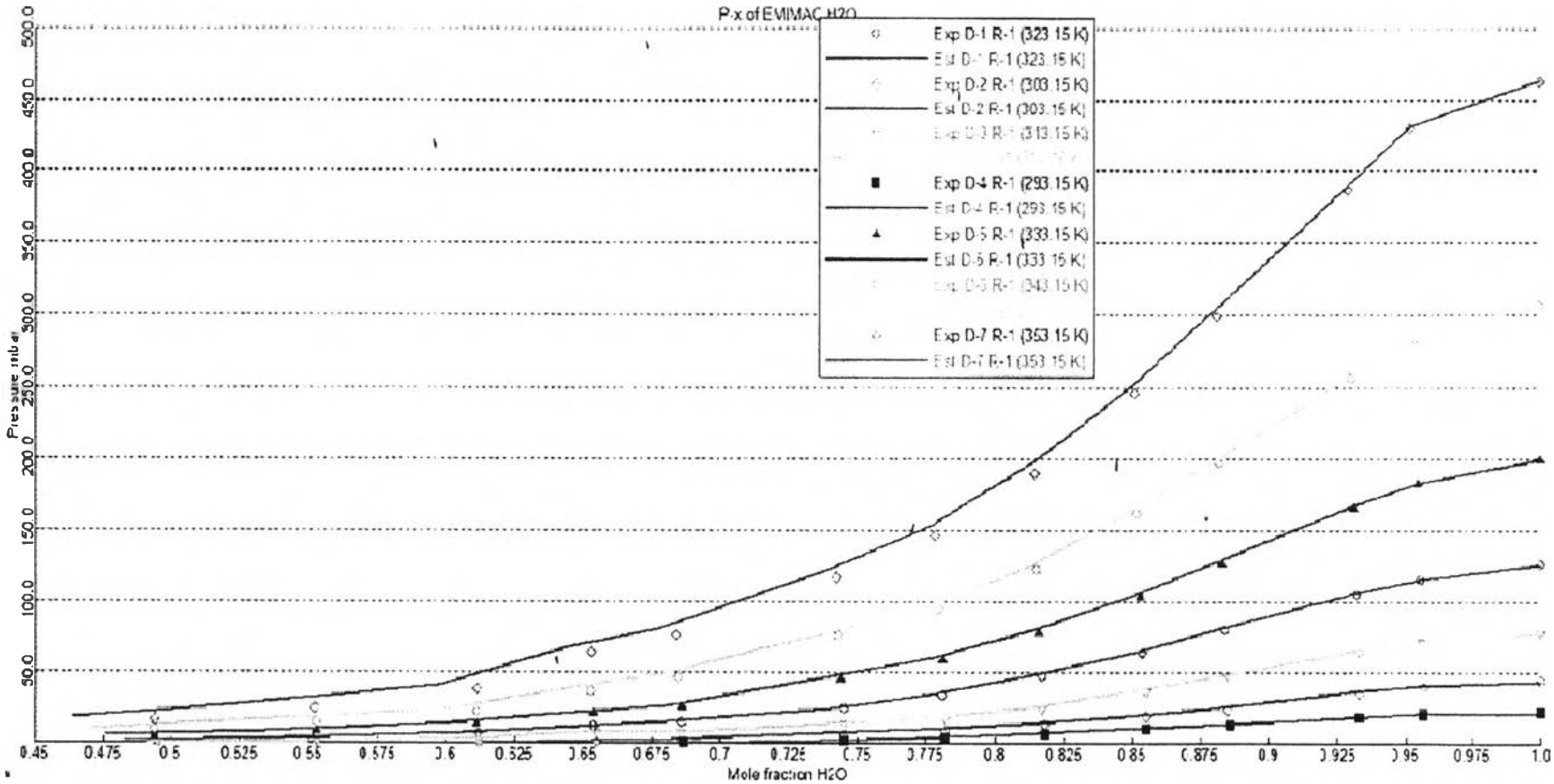


Figure C1 Comparison of isothermal solubility data of H_2O in ionic liquid [emim][Ac] between the experiment and regression, at 293.15, 303.15, 313.15, 323.15, 333.15, 343.15, and 353.15K. Line represents the estimations by the NRTL. (From the Aspen program)

Appendix C2: Henry's Constant Mode

The Henry's law constant model-Aspen is used to calculate K-value for dissolved gas components (CO_2, N_2) in the mixture. Henry's law is available in all activity coefficient model methods. The general equation of Henry's constant of the Aspen is shown as:

$$\ln H_{iA}(T, p_A^{*,l}) = a_{iA} + b_{iA}/T + c_{iA}\ln T + d_{iA}T + e_{iA}/T^2 \quad \text{for } T_L \le T \le T_H$$

Henry's Constant of CO_2 in [emim][Ac]

Ref: Phase Behavior of Carbon Dioxide in Ionic Liquids: [emim][Acetate], [emim][Trifluoroacetate], and [emim][Acetate] + [emim][Trifluoroacetate] Mixtures; Mark B. Shiflett, and A. Yokozeki

Table C2.1 Henry's constant (NRTL) of the binary system for CO2 and ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (SI-unit/K)
HENRY/1	aij	-958.843
HENRY/2	bij	-10000
HENRY/3	cij	171.3431
HENRY/4	dij	0
HENRY/5	Tlower	0
HENRY/6	Tupper	2000
HENRY/7	eij	0

Note: I = solute(CO_2), A = solvent [emim][Ac].

Table C2.2 Mole-fraction of CO_2 in binary mixture at a constant temperature 298.1 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
298.1	0.01	0.010454	0.189	0.191734	1.446349
298.1	0.0499	0.051456	0.246	0.249665	1.489959
298.1	0.1	0.102478	0.267	0.27077	1.411835
298.1	0.3996	0.404424	0.313	0.316569	1.140383
298.1	0.6995	0.704516	0.34	0.343407	1.002029
298.1	0.9996	1.003757	0.362	0.365264	0.90174
298.1	1.2998	1.302503	0.384	0.387176	0.827161
298.1	1.4997	1.501178	0.398	0.401117	0.783191
298.1	1.9998	1.997395	0.428	0.430887	0.674626
				AAD (%)	0.263892

Table C2.3 Mole-fraction of CO_2 in binary mixture at a constant temperature 323.1 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
323.1	0.01	0.010517	0.138	0.139012	0.733551
323.1	0.0499	0.051831	0.203	0.204886	0.928916
323.1	0.1	0.103271	0.23	0.232161	0.939522
323.1	0.4	0.408196	0.285	0.287342	0.82186
323.1	0.7	0.710994	0.314	0.316331	0.742197
323.1	1.0001	1.01283	0.336	0.338283	0.679524
323.1	1.2997	1.313291	0.35	0.352128	0.607943
323.1	1.4998	1.513758	0.361	0.363079	0.575873
323.1	1.9996	2.0139	0.39	0.392022	0.518538
				AAD (%)	0.117402

Table C2.4 Mole-fraction of CO_2 in binary mixture at a constant temperature 348.2 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
348.2	0.0101	0.010669	0.094	0.094062	0.065426
348.2	0.0501	0.052344	0.157	0.157481	0.306051
348.2	0.1002	0.104135	0.186	0.186683	0.367151
348.2	0.3997	0.41069	0.241	0.24183	0.34444
348.2	0.6996	0.715432	0.264	0.264749	0.283598
348.2	0.9998	1.019342	0.28	0.280647	0.231179
348.2	1.2996	1.322139	0.294	0.294561	0.190782
348.2	1.4997	1.523708	0.298	0.298447	0.149899
348.2	1.9996	2.027225	0.321	0.321365	0.113707
				AAD (%)	0.087175

Table C2.5 Average absolute deviation (AAD %) between experimental and estimated value of mole fraction by the Henry's constant for the [emim][Ac] + CO_2 system

	Temperature (K)			Average AAD (%)
	298.1	323.1	348.2	
AAD (%)	0.028003	0.0258	0.017558	0.023787

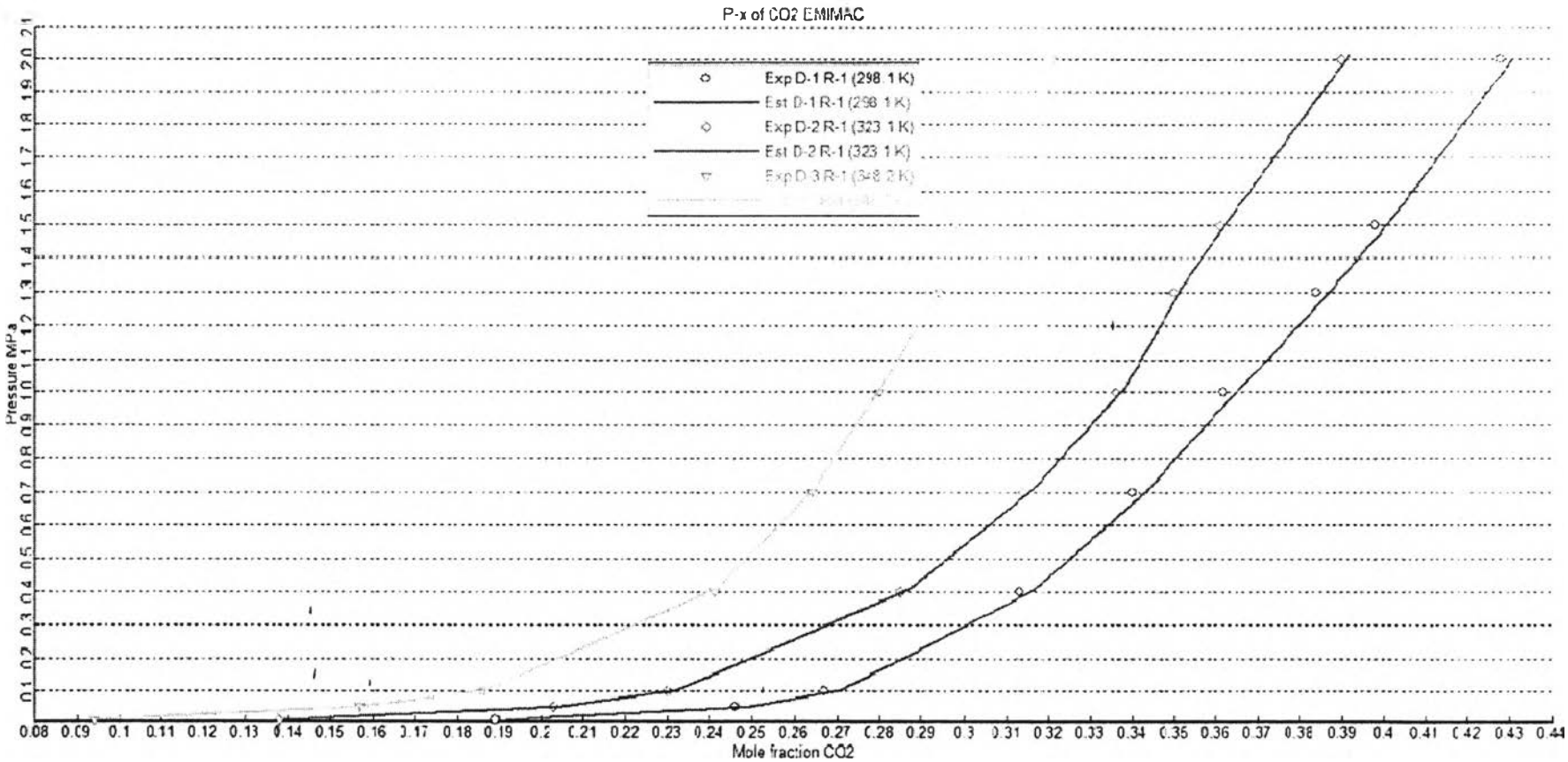


Figure C2.1 Comparison of isothermal solubility data of CO_2 in ionic liquid [emim][Ac] between the experiment and regression, at 298.1, 323.1, and 348.2 K. Line represents the estimations by the Henry's constant model. (From the Aspen program)

Henry's Constant of N_2 in [emim][Ac]

Ref: Solubility of carbon dioxide, ethane, methane, oxygen, nitrogen, hydrogen, argon, and carbon monoxide in 1-butyl-3-methylimidazolium tetrafluoroborate between temperatures 283 K and 343 K and at pressures close to atmospheric ; Johan Jacquemin, Margarida F. Costa Gomes , Pascale Husson, Vladimir Majer.

Table C2.6 Henry's constant (NRTL) of the binary system for N_2 and ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (SI-unit/K)
HENRY/1	aij	-212.899
HENRY/2	bij	9377.806
HENRY/3	cij	33.61916
HENRY/4	dij	0
HENRY/5	Tlower	0
HENRY/6	Tupper	2000
HENRY/7	eij	0

Note: I = solute (N_2), j = solvent [emim][Ac].

Table C2.7 Mole-fraction of N_2 in binary mixture at a constant pressure 0.1 MPa

Pressure (MPa) (constant)	Temperature (K)		Mole fraction of N_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
0.1	283.2	283.1846	0.000634	0.000633	-0.08678
0.1	293.21	293.2985	0.000608	0.000609	0.156353
0.1	303.3867	303.7019	0.000561	0.000563	0.34778
0.1	313.29	312.3526	0.000525	0.000521	-0.81143
0.1	323.245	323.6976	0.000443	0.000444	0.314018
0.1	333.245	333.6925	0.000379	0.00038	0.268952
0.1	343.14	342.789	0.000326	0.000326	-0.19301
				AAD (%)	0.311273

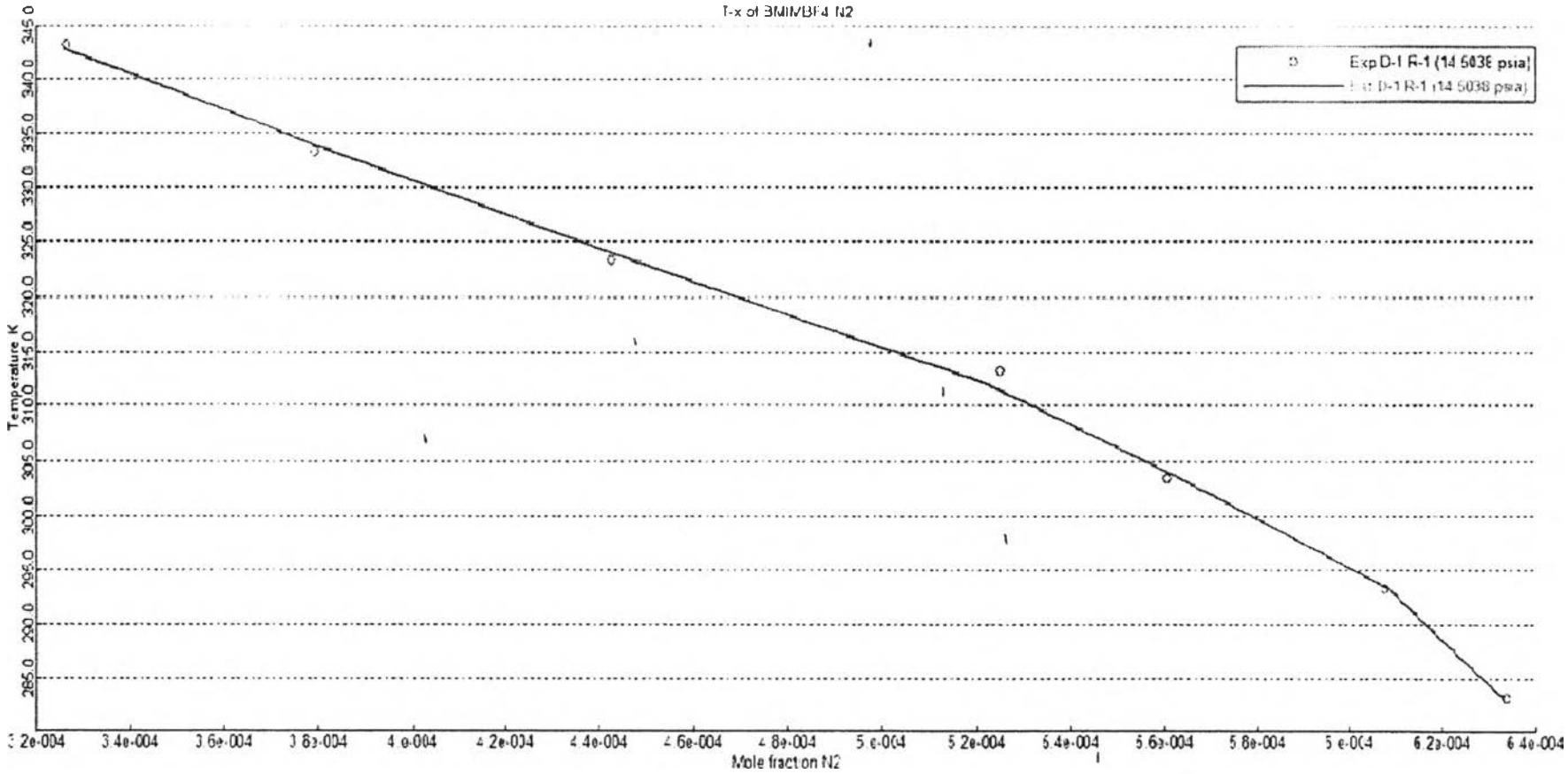


Figure C2.2 Comparison of isobaric solubility data of N_2 in ionic liquid [emim][Ac] between the experiment and regression at 0.1 MPa. Line represents the estimations by the Henry's constant model. (From the Aspen program)

Appendix C3: The Standard Peng-Robinson (PRBM)

I also used The Standard Peng-Robinson (PRBM) and the Redlich-Kwong-Aspen (The SRK with quadratic mixing rules) equation of state to predict the P-x diagram of the binary system of CO_2 and ionic liquid [emim][Ac].

Ref: Phase Behavior of Carbon Dioxide in Ionic Liquids: [emim][Acetate], [emim][Trifluoroacetate], and [emim][Acetate] + [emim][Trifluoroacetate] Mixtures; Mark B. Shiflett, and A. Yokozeki.

The equation for this model:

$$p = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m + b) + b(V_m - b)}$$

Where:

$$b = \sum_i x_i b_i$$

$$a = \sum_i \sum_j x_i x_j (a_i a_j)^{0.5} (1 - k_{ij})$$

$$a_i = fcn(T, T_{ci}, p_{ci}, \omega_i)$$

$$b_i = fcn(T_{ci}, p_{ci})$$

$$k_{ij} = k_{ij}^{(1)} + k_{ij}^{(2)} T + k_{ij}^{(3)} / T$$

$$k_{ij} = k_{ji}$$

Table C3.1 The binary interaction parameters (PRBM) of the binary system for CO_2 and ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (SI-unit/K)		Tempreature (K)	k_{12}
PRKBV/1	kaij	-74.9236		298.1	-0.44913
PRKBV/2	kbij	0.137299		323.1	0.387714
PRKBV/3	kcij	10000		348.2	1.602867
PRKBV/4	Tlower	1.26E-08			
PRKBV/5	Tuppper	1000			

Note: I = solute CO_2, j = solvent [emim][Ac].

Note: k_{12} = -74.9236 + (0.137299 x T(K)) + (10000/T(K)).

Table C3.2 Mole-fraction of CO2 in binary mixture at a constant temperature 298.1 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO2		%AAD
	Experiment	Regression	Experiment	Regression	
298.1	0.01	0.010133	0.189	0.193185	2.214074
298.1	0.0499	0.050301	0.246	0.251625	2.286382
298.1	0.1	0.100517	0.267	0.272927	2.219925
298.1	0.3996	0.399018	0.313	0.319595	2.107093
298.1	0.6995	0.696073	0.34	0.347389	2.173235
298.1	0.9996	0.991699	0.362	0.370273	2.285221
298.1	1.2998	1.28541	0.384	0.393383	2.443568
298.1	1.4997	1.479633	0.398	0.408191	2.560528
298.1	1.9998	1.959809	0.428	0.440135	2.835327
				%AAD	0.177253

Table C3.3 Mole-fraction of CO_2 in binary mixture at a constant temperature 323.1 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
323.1	0.01	0.010306	0.138	0.138524	0.379783
323.1	0.0499	0.051109	0.203	0.204211	0.596404
323.1	0.1	0.102089	0.23	0.231494	0.649348
323.1	0.4	0.405099	0.285	0.287155	0.75614
323.1	0.7	0.70575	0.314	0.316742	0.873248
323.1	1.0001	1.00434	0.336	0.339332	0.991518
323.1	1.2997	1.300127	0.35	0.353738	1.067971
323.1	1.4998	1.496131	0.361	0.365102	1.13615
323.1	1.9996	1.979052	0.39	0.395196	1.332308
				AAD (%)	0.239417

Table C3.4 Mole-fraction of CO_2 in binary mixture at a constant temperature 348.2 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
348.2	0.0101	0.010561	0.094	0.09302	-1.04213
348.2	0.0501	0.052058	0.157	0.15566	-0.85338
348.2	0.1002	0.103762	0.186	0.18456	-0.77435
348.2	0.3997	0.410241	0.241	0.239554	-0.59983
348.2	0.6996	0.714331	0.264	0.262676	-0.50144
348.2	0.9998	1.01628	0.28	0.278805	-0.42693
348.2	1.2996	1.315223	0.294	0.292928	-0.36463
348.2	1.4997	1.513278	0.298	0.296947	-0.35322
348.2	1.9996	2.001188	0.321	0.32012	-0.27424
				AAD (%)	0.213991

Table C3.5 Average absolute deviation (AAD %) between experimental and estimated value of mole fraction by the for the [emim][Ac] + CO_2 system

	Temperature (K)			Average AAD (%)
	298.1	323.1	348.2	
AAD (%)	0.213991	0.239417	0.177253	0.210221

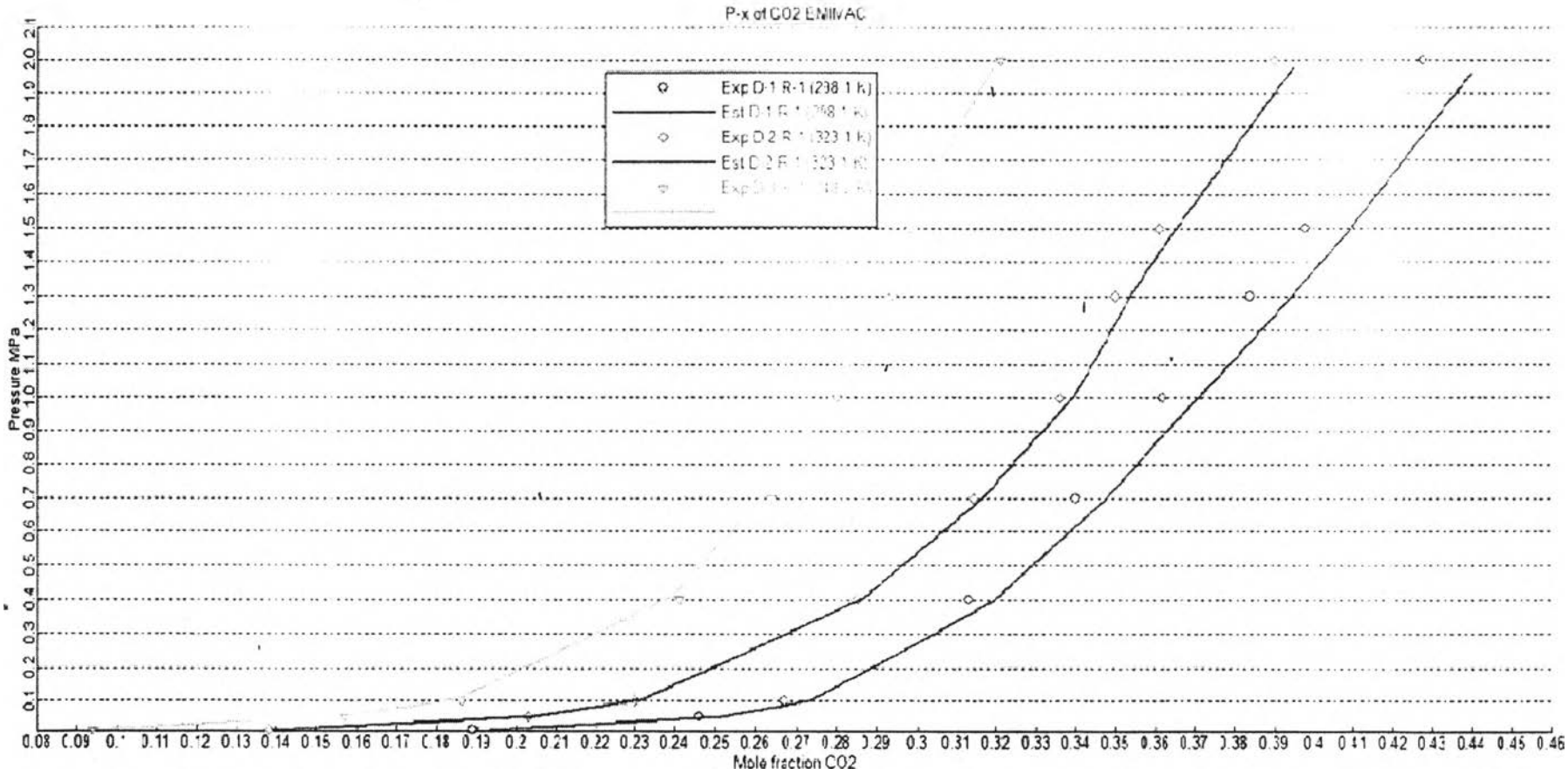


Figure C3 Comparison of isothermal solubility data of CO_2 in ionic liquid [emim][Ac] between the experiment and regression, at 298.1, 323.1, and 348.2 K. Line represents the estimations by the Standard Peng-Robinson (PRBM). (From the Aspen program)

Appendix C4:The Redlich-Kwong-Aspen (SRK)

The equation for this model:

$$p = \frac{RT}{V_m - b} - \frac{a}{V_m(V_m + b)}$$

A quadratic mixing rule is maintained for:

$$a = \sum_i \sum_j x_i x_j (a_i a_j)^{0.5} (1 - k_{a,ij})$$

An interaction parameter is introduced in the mixing rule for:

$$b = \sum_i \sum_j x_i x_j \frac{(b_i + b_j)}{2} (1 - k_{b,ij})$$

For a_i an extra polar parameter is used:

$$a_i = fcn(T, T_{ci}, p_{ci}, \omega_i, \eta_i)$$

$$b_i = fcn(T_{ci}, p_{ci})$$

The interaction parameters are temperature-dependent:

$$k_{a,ij} = k^0_{a,ij} + k^1_{a,ij} \frac{T}{1000}$$

$$k_{b,ij} = k^0_{b,ij} + k^1_{b,ij} \frac{T}{1000}$$

Table 4.1 The binary interaction parameters (SRK) of the binary system for CO_2 and ionic liquid [emim][Ac] from regression

Parameter/ Name	Symbol	Value (SI-unit/K)		Temperature (K)	$k_{a,12}$	$k_{b,12}$
RKAKA0	ka,ij0	-25.6437		298.1	-11.4901	-4.18122
RKAKA1	ka,ij1	47.4795		323.1	-10.3031	-3.72645
RKAKB0	kb,ij0	-9.60394		348.2	-9.11134	-3.26986
RKAKB1	kb,ij1	18.19093				

Note: I = CO_2, [emim][Ac]; j = CO_2, [emim][Ac]

Note: $k_{a,ij}$ = -25.6437 + (47.4795*T(K)).

$k_{b,ij}$ = -9.60394 + (18.19093*T(K)).

Table 4.2 Mole-fraction of CO_2 in binary mixture at a constant temperature 298.1 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
298.1	0.01	0.010266	0.189	0.191703	14.30159
298.1	0.0499	0.050173	0.246	0.251859	23.81504
298.1	0.1	0.100238	0.267	0.276536	35.7161
298.1	0.3996	0.397606	0.313	0.322901	31.63291
298.1	0.6995	0.692862	0.34	0.34713	20.97088
298.1	0.9996	0.986733	0.362	0.367242	14.48039
298.1	1.2998	1.280329	0.384	0.387985	10.37682
298.1	1.4997	1.476101	0.398	0.40156	8.944724
298.1	1.9998	1.96798	0.428	0.431903	9.117991
				AAD (%)	8.192312

Table 4.3 Mole-fraction of CO_2 in binary mixture at a constant temperature 323.1 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
323.1	0.01	0.01116	0.138	0.117248	-15.0377
323.1	0.0499	0.051263	0.203	0.204608	0.792315
323.1	0.1	0.102384	0.23	0.233126	1.359087
323.1	0.4	0.407004	0.285	0.279277	-2.00818
323.1	0.7	0.708067	0.314	0.30043	-4.32169
323.1	1.0001	1.005531	0.336	0.318069	-5.33652
323.1	1.2997	1.299155	0.35	0.330747	-5.50089
323.1	1.4998	1.494313	0.361	0.341624	-5.36729
323.1	1.9996	1.982372	0.39	0.37223	-4.55654
				AAD (%)	3.019835

Table 4.4 Mole-fraction of CO_2 in binary mixture at a constant temperature 348.2 K

Temperature (K) (constant)	Pressure (MPa)		Mole fraction of CO_2		AAD (%)
	Experiment	Regression	Experiment	Regression	
348.2	0.0101	0.010126	0.094	0.100574	6.993511
348.2	0.0501	0.050597	0.157	0.188723	20.20599
348.2	0.1002	0.102883	0.186	0.213416	14.73989
348.2	0.3997	0.416139	0.241	0.25421	5.481328
348.2	0.6996	0.724497	0.264	0.27293	3.382727
348.2	0.9998	1.01944	0.28	0.283778	1.349179
348.2	1.2996	1.297831	0.294	0.289409	-1.5616
348.2	1.4997	1.47458	0.298	0.289608	-2.81601
348.2	1.9996	1.888354	0.321	0.291722	-9.12075
				AAD (%)	6.720232

Table 4.5 Average absolute deviation (AAD %) between experimental and estimated value of mole fraction by the for the [emim][Ac] + CO_2 system

	Temperature (K)			Average AAD (%)
	298.1	323.1	348.2	
AAD (%)	8.192312	3.019835	6.720232	5.97746

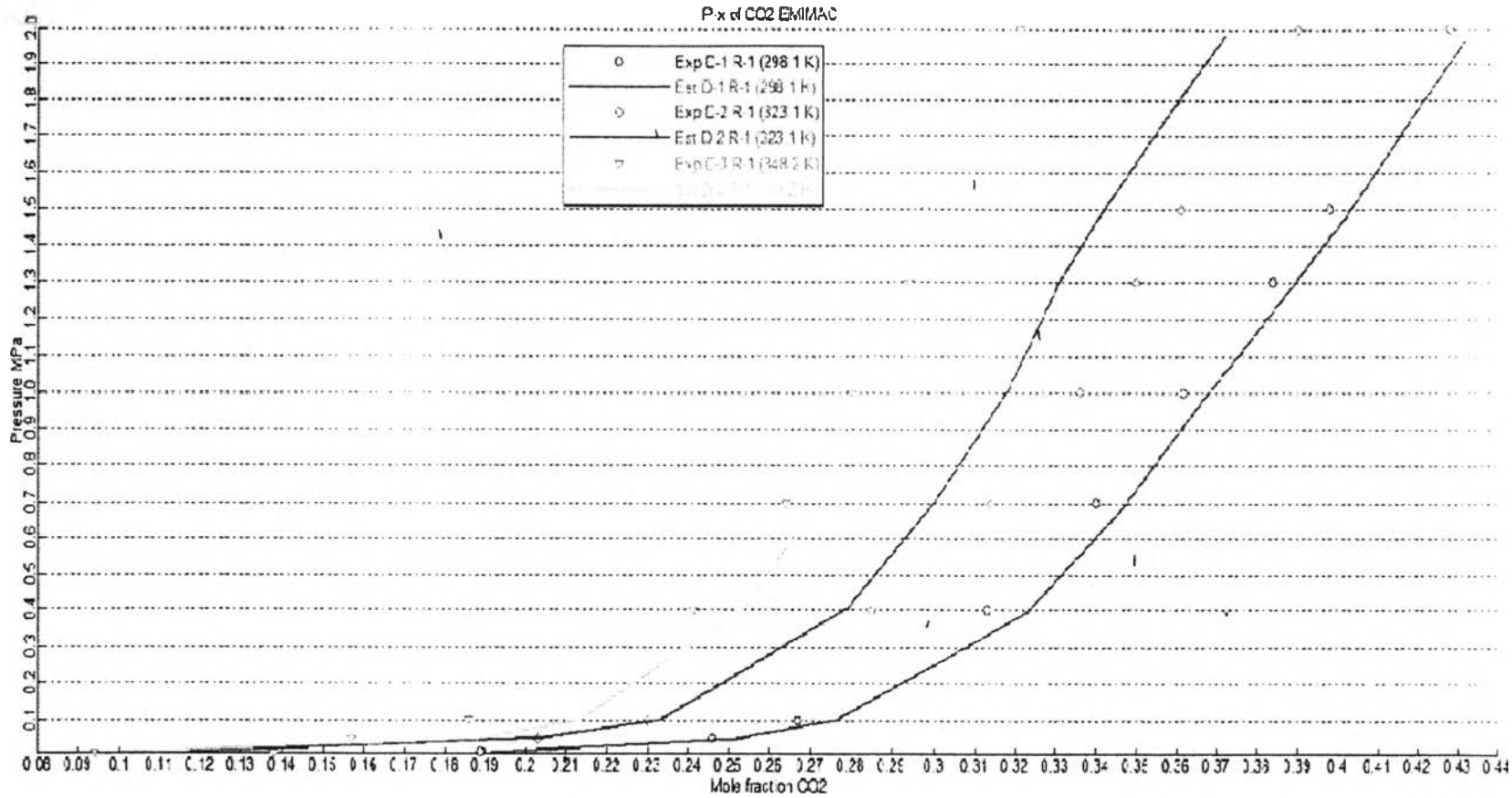


Figure C4 Comparison of isothermal solubility data of CO_2 in ionic liquid [emim][Ac] between the experiment and regression, at 298.1, 323.1, and 348.2 K. Line represents the estimations by the Redlich-Kwong-Aspen (SRK). (From the Aspen program)

Appendix D: Equilibrium Model

Carbon dioxide solubility in ionic liquid [emim][Ac] show extremely unusual phase behavior, CO_2 dissolve in the ionic liquid at a large concentration (up to about 20 mol % of CO_2 with almost no vapor pressure above the mixture. This result is similar to [bmim][Ac] and [eemim][Ac]. In all three cases the CO_2 forms the molecular complexes (or chemical reaction) with ionic liquid. NMR spectroscopy has identified the structure imidazoilum-2-carboxylate. Shiflett *et al.* (2010) proposed the equilibrium calculation based on their experiment measurement (CO_2 + [bmim][Ac]), 2010. Due to the similarity of CO_2 absorption behaviors between [bmim][Ac], [emim][Ac] ,and [eemim][Ac]. The equilibrium calculation of [emim][Ac] is set equal to as [bmim][Ac].

Ref: Carbon Dioxide Capture Using Ionic Liquid 1-Butyl-3-methylimidazolium Acetate ;Mark B. Shiflett, David W. Drew, Robert A. Cantini, and A. Yokozeki, Phase Behavior of CO_2 in Room-temperature Ionic Liquid 1-Ethyl-3-Ethylimidazolium Acetate; Shiflett MB, Elliot BA, Lustiq SR,Sabesan S, Kelkar MS, Yokozeki A.

Reaction

Rxn1: emimAc + CO2 = emimCO2
Rxn2: emimCO2 + emimAc = emim2CO2
Rxn3; emim2CO2 + emimAc = emim3CO2

Rxn1: Keq = [emimCO2] / [emimAc]*[CO2]
Rxn2: Keq = [emim2CO2] / [emimAc]*[emimCO2]
Rxn3: Keq = [emim3CO2] / [emimAc]*[emim2CO2]
(in mole fraction)

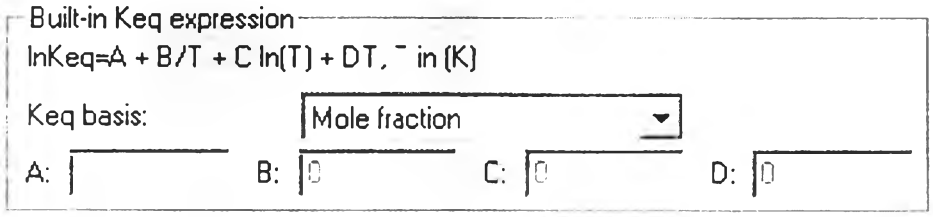


Table D4.1 Equilibrium parameter of the reaction system of CO_2 and [emim][Ac]'

Reaction	Stoichiometry					Equilibrium parameters	
	CO_2	emimAc	$emimCO_2$	$emim_2CO_2$	$emim_3CO_2$	A	B
1	-1	-1	1			-6.5655	2743.9
2		-1	-1	1		7.6412	-1942.5
3		-1		-1	1	-0.7193	531.27

Table D4.2 Composition at equilibrium at a range of temperature from 273.15 to 468.15 K

Temperature (K)	Equilibrium constant (Keq)			Temperature (K)	Equilibrium constant (Keq)		
	Rxn1	Rxn2	Rxn1		Rxn1	Rxn2	Rxn3
273.15	32.45636	1.698461	3.406466	373.15	2.198649	11.42174	2.022721
278.15	27.09424	1.930073	3.289424	378.15	1.994943	12.2356	1.985
283.15	22.7627	2.18339	3.180329	383.15	1.814709	13.08392	1.948939
288.15	19.23961	2.459405	3.078453	388.15	1.65479	13.96692	1.914437
293.15	16.35534	2.759086	2.983152	393.15	1.512509	14.88476	1.8814
298.15	13.97941	3.08337	2.893851	398.15	1.385587	15.83758	1.849742
303.15	12.01066	3.43316	2.81004	403.15	1.272078	16.82548	1.819383
308.15	10.37013	3.809324	2.73126	408.15	1.170316	17.84852	1.790247
313.15	8.99577	4.212694	2.6571	413.15	1.078869	18.90673	1.762267
318.15	7.838505	4.644062	2.587191	418.15	0.996505	20.00011	1.735377
323.15	6.859285	5.104179	2.521201	423.15	0.922158	21.12864	1.709519

328.15	6.026852	5.593756	2.458829	428.15	0.854905	22.29224	1.684637
333.15	5.316047	6.113461	2.399804	433.15	0.793943	23.49084	1.660679
338.15	4.706508	6.66392	2.34388	438.15	0.738575	24.72431	1.637597
343.15	4.181674	7.245715	2.290832	443.15	0.688189	25.99251	1.615346
348.15	3.728004	7.859385	2.240458	448.15	0.642253	27.29528	1.593884
353.15	3.334378	8.505427	2.192571	453.15	0.600297	28.63243	1.573171
358.15	2.99162	9.184294	2.147003	458.15	0.56191	30.00375	1.553171
363.15	2.692125	9.896396	2.103598	463.15	0.526729	31.409	1.533848
368.15	2.429564	10.6421	2.062214	468.15	0.494433	32.84794	1.515171

Appendix E: Aspen Plus® Input Files for MEA Process

Input Summary

ASPEN Plus® Input Files for MEA and Ionic Liquid Processes

MEA Process:

```
;
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with utilities  Filename C:\Users\ADMINI~1\AppData\Local\Temp\~ap1dc3.tmp
;


DYNAMICS
   DYNAMICS RESULTS=ON

TITLE 'MEA'

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
      VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'  &
      MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
      MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l'  &
      PDROP=bar

DEF-STREAMS CONVEN ALL

SIM-OPTIONS OLD-DATABANK=YES

DESCRIPTION "
   Electrolytes Simulation with Metric Units :
   C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr.

   Property Method: ELECNRTL

   Flow basis for input: Mass

   Stream report composition: Mass flow
   "

DATABANKS ASPENPCD / AQUEOUS / SOLIDS / INORGANIC / &
      PURE22

PROP-SOURCES ASPENPCD / AQUEOUS / SOLIDS / INORGANIC / &
      PURE22
```

```
COMPONENTS
   H2O H2O /
   CO2 CO2 /
   N2 N2 /
   MONOE-01 C2H7NO /
   MEA+ C2H8NO+ /
   H3O+ H3O+ /
   MEACOO- C3H6NO3- /
   HCO3- HCO3- /
   OH- OH- /
   CO3-- CO3-2

HENRY-COMPS GLOBAL CO2 N2

CHEMISTRY GLOBAL
   STOIC 1 H2O -2 / H3O+ 1 / OH- 1
   STOIC 2 CO2 -1 / H2O -2 / H3O+ 1 / HCO3- 1
   STOIC 3 HCO3- -1 / H2O -1 / H3O+ 1 / CO3-- 1
   STOIC 4 MEA+ -1 / H2O -1 / MONOE-01 1 / H3O+ 1
   STOIC 5 MEACOO- -1 / H2O -1 / MONOE-01 1 / HCO3- 1
   K-STOIC 1 A=132.89888 B=-13445.9 C=-22.4773 D=0
   K-STOIC 2 A=231.465439 B=-12092.1 C=-36.7816 D=0
   K-STOIC 3 A=216.050446 B=-12431.7 C=-35.4819 D=0
   K-STOIC 4 A=-3.038325 B=-7008.357 C=0 D=-.00313489
   K-STOIC 5 A=-.52135 B=-2545.53 C=0 D=0

FLOWSHEET
   BLOCK SCRUBBER IN=FLUEGAS 4 OUT=SCRUBGAS 2
   BLOCK ABSORBER IN=SCRUBGAS XLEANOIL OUT=ABSVENT RICHOIL
   BLOCK B1 IN=RICHOIL OUT=1
   BLOCK B2 IN=16 OUT=3
   BLOCK B3 IN=3 10 OUT=5 6
   BLOCK B4 IN=5 OUT=7
   BLOCK B5 IN=7 OUT=8 9
   BLOCK B6 IN=9 OUT=10
   BLOCK B7 IN=6 OUT=11
   BLOCK B8 IN=17 OUT=12
   BLOCK B9 IN=12 MEAMK H2OMK OUT=14
   BLOCK CROSSHX IN=11 1 OUT=17 16
   BLOCK B13 IN=14 OUT=18 19
   BLOCK B14 IN=19 20 OUT=21
   BLOCK B10 IN=13 15 OUT=22 23
   BLOCK B11 IN=24 29 OUT=25 30
   BLOCK B12 IN=25 OUT=26
   BLOCK B15 IN=26 OUT=27 28
   BLOCK B16 IN=28 OUT=29
```

```
PROPERTIES ELECNRTL HENRY-COMPS=GLOBAL CHEMISTRY=GLOBAL
&
     TRUE-COMPS=YES

PROP-DATA HENRY-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST HENRY
  BPVAL CO2 H2O 159.1996745 -8477.711000 -21.95743000 &
    5.78074800E-3 -.1500000000 226.8500000 0.0
  BPVAL N2 H2O 164.9940745 -8432.770000 -21.55800000 &
    -8.4362400E-3 -.1500000000 72.85000000 0.0

PROP-DATA NRTL-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST NRTL
  BPVAL H2O CO2 10.06400000 -3268.135000 .2000000000 0.0 0.0 &
    0.0 0.0 200.0000000
  BPVAL CO2 H2O 10.06400000 -3268.135000 .2000000000 0.0 0.0 &
    0.0 0.0 200.0000000
  BPVAL H2O MONOE-01 1.438498000 99.02104000 .2000000000 0.0 &
    0.0 0.0 25.00000000 150.0000000
  BPVAL MONOE-01 H2O -1.046602000 -337.5456000 .2000000000 &
    0.0 0.0 0.0 25.00000000 150.0000000

PROP-DATA VLCLK-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST VLCLK
  BPVAL MEA+ OH- -390.9954000 1000.000000

PROP-DATA GMELCC-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
```

```
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'  &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l'  &
    PDROP=bar

PROP-LIST GMELCC
  PPVAL H2O ( MEA+ MEACOO- ) 9.887700000
  PPVAL ( MEA+ MEACOO- ) H2O -4.951100000
  PPVAL H2O ( MEA+ HCO3- ) 5.354100000
  PPVAL ( MEA+ HCO3- ) H2O -4.070500000
  PPVAL H2O ( H3O+ HCO3- ) 8.045000000
  PPVAL ( H3O+ HCO3- ) H2O -4.072000000
  PPVAL H2O ( H3O+ OH- ) 8.045000000
  PPVAL ( H3O+ OH- ) H2O -4.072000000
  PPVAL H2O ( H3O+ CO3-- ) 8.045000000
  PPVAL ( H3O+ CO3-- ) H2O -4.072000000
  PPVAL CO2 ( MEA+ MEACOO- ) 15.00000000
  PPVAL ( MEA+ MEACOO- ) CO2 -8.000000000
  PPVAL CO2 ( MEA+ HCO3- ) 15.00000000
  PPVAL ( MEA+ HCO3- ) CO2 -8.000000000
  PPVAL CO2 ( MEA+ OH- ) 15.00000000
  PPVAL ( MEA+ OH- ) CO2 -8.000000000
  PPVAL CO2 ( MEA+ CO3-- ) 15.00000000
  PPVAL ( MEA+ CO3-- ) CO2 -8.000000000
  PPVAL CO2 ( H3O+ MEACOO- ) 15.00000000
  PPVAL ( H3O+ MEACOO- ) CO2 -8.000000000
  PPVAL CO2 ( H3O+ HCO3- ) 15.00000000
  PPVAL ( H3O+ HCO3- ) CO2 -8.000000000
  PPVAL CO2 ( H3O+ OH- ) 15.00000000
  PPVAL ( H3O+ OH- ) CO2 -8.000000000
  PPVAL CO2 ( H3O+ CO3-- ) 15.00000000
  PPVAL ( H3O+ CO3-- ) CO2 -8.000000000
  PPVAL MONOE-01 ( MEA+ MEACOO- ) 15.00000000
  PPVAL ( MEA+ MEACOO- ) MONOE-01 -8.000000000
  PPVAL MONOE-01 ( MEA+ HCO3- ) 15.00000000
  PPVAL ( MEA+ HCO3- ) MONOE-01 -8.000000000
  PPVAL MONOE-01 ( MEA+ OH- ) 15.00000000
  PPVAL ( MEA+ OH- ) MONOE-01 -8.000000000
  PPVAL MONOE-01 ( MEA+ CO3-- ) 15.00000000
  PPVAL ( MEA+ CO3-- ) MONOE-01 -8.000000000
  PPVAL MONOE-01 ( H3O+ MEACOO- ) 15.00000000
  PPVAL ( H3O+ MEACOO- ) MONOE-01 -8.000000000
  PPVAL MONOE-01 ( H3O+ HCO3- ) 15.00000000
  PPVAL ( H3O+ HCO3- ) MONOE-01 -8.000000000
  PPVAL MONOE-01 ( H3O+ OH- ) 15.00000000
  PPVAL ( H3O+ OH- ) MONOE-01 -8.000000000
```

```
  PPVAL MONOE-01 ( H3O+ CO3-- ) 15.00000000
  PPVAL ( H3O+ CO3-- ) MONOE-01 -8.000000000

PROP-DATA GMELCD-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST GMELCD
  PPVAL H2O ( MEA+ MEACOO- ) 10.81300000
  PPVAL ( MEA+ MEACOO- ) H2O 0.0
  PPVAL H2O ( MEA+ HCO3- ) 965.2400000
  PPVAL ( MEA+ HCO3- ) H2O -11.06700000
  PPVAL CO2 ( MEA+ MEACOO- ) 0.0
  PPVAL ( MEA+ MEACOO- ) CO2 0.0
  PPVAL CO2 ( MEA+ HCO3- ) 0.0
  PPVAL ( MEA+ HCO3- ) CO2 0.0
  PPVAL CO2 ( MEA+ OH- ) 0.0
  PPVAL ( MEA+ OH- ) CO2 0.0
  PPVAL CO2 ( MEA+ CO3-- ) 0.0
  PPVAL ( MEA+ CO3-- ) CO2 0.0
  PPVAL CO2 ( H3O+ MEACOO- ) 0.0
  PPVAL ( H3O+ MEACOO- ) CO2 0.0
  PPVAL CO2 ( H3O+ HCO3- ) 0.0
  PPVAL ( H3O+ HCO3- ) CO2 0.0
  PPVAL CO2 ( H3O+ OH- ) 0.0
  PPVAL ( H3O+ OH- ) CO2 0.0
  PPVAL CO2 ( H3O+ CO3-- ) 0.0
  PPVAL ( H3O+ CO3-- ) CO2 0.0
  PPVAL MONOE-01 ( MEA+ MEACOO- ) 0.0
  PPVAL ( MEA+ MEACOO- ) MONOE-01 0.0
  PPVAL MONOE-01 ( MEA+ HCO3- ) 0.0
  PPVAL ( MEA+ HCO3- ) MONOE-01 0.0
  PPVAL MONOE-01 ( MEA+ OH- ) 0.0
  PPVAL ( MEA+ OH- ) MONOE-01 0.0
  PPVAL MONOE-01 ( MEA+ CO3-- ) 0.0
  PPVAL ( MEA+ CO3-- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ MEACOO- ) 0.0
  PPVAL ( H3O+ MEACOO- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ HCO3- ) 0.0
  PPVAL ( H3O+ HCO3- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ OH- ) 0.0
  PPVAL ( H3O+ OH- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ CO3-- ) 0.0
  PPVAL ( H3O+ CO3-- ) MONOE-01 0.0
```

```
PROP-DATA GMELCE-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST GMELCE
  PPVAL CO2 ( MEA+ MEACOO- ) 0.0
  PPVAL ( MEA+ MEACOO- ) CO2 0.0
  PPVAL CO2 ( MEA+ HCO3- ) 0.0
  PPVAL ( MEA+ HCO3- ) CO2 0.0
  PPVAL CO2 ( MEA+ OH- ) 0.0
  PPVAL ( MEA+ OH- ) CO2 0.0
  PPVAL CO2 ( MEA+ CO3-- ) 0.0
  PPVAL ( MEA+ CO3-- ) CO2 0.0
  PPVAL CO2 ( H3O+ MEACOO- ) 0.0
  PPVAL ( H3O+ MEACOO- ) CO2 0.0
  PPVAL CO2 ( H3O+ HCO3- ) 0.0
  PPVAL ( H3O+ HCO3- ) CO2 0.0
  PPVAL CO2 ( H3O+ OH- ) 0.0
  PPVAL ( H3O+ OH- ) CO2 0.0
  PPVAL CO2 ( H3O+ CO3-- ) 0.0
  PPVAL ( H3O+ CO3-- ) CO2 0.0
  PPVAL MONOE-01 ( MEA+ MEACOO- ) 0.0
  PPVAL ( MEA+ MEACOO- ) MONOE-01 0.0
  PPVAL MONOE-01 ( MEA+ HCO3- ) 0.0
  PPVAL ( MEA+ HCO3- ) MONOE-01 0.0
  PPVAL MONOE-01 ( MEA+ OH- ) 0.0
  PPVAL ( MEA+ OH- ) MONOE-01 0.0
  PPVAL MONOE-01 ( MEA+ CO3-- ) 0.0
  PPVAL ( MEA+ CO3-- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ MEACOO- ) 0.0
  PPVAL ( H3O+ MEACOO- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ HCO3- ) 0.0
  PPVAL ( H3O+ HCO3- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ OH- ) 0.0
  PPVAL ( H3O+ OH- ) MONOE-01 0.0
  PPVAL MONOE-01 ( H3O+ CO3-- ) 0.0
  PPVAL ( H3O+ CO3-- ) MONOE-01 0.0

PROP-DATA GMELCN-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
```

```
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST GMELCN
  PPVAL CO2 ( MEA+ MEACOO- ) .1000000000
  PPVAL CO2 ( MEA+ HCO3- ) .1000000000
  PPVAL CO2 ( MEA+ OH- ) .1000000000
  PPVAL CO2 ( MEA+ CO3-- ) .1000000000
  PPVAL CO2 ( H3O+ MEACOO- ) .1000000000
  PPVAL CO2 ( H3O+ HCO3- ) .1000000000
  PPVAL CO2 ( H3O+ OH- ) .1000000000
  PPVAL CO2 ( H3O+ CO3-- ) .1000000000
  PPVAL MONOE-01 ( MEA+ MEACOO- ) .1000000000
  PPVAL MONOE-01 ( MEA+ HCO3- ) .1000000000
  PPVAL MONOE-01 ( MEA+ OH- ) .1000000000
  PPVAL MONOE-01 ( MEA+ CO3-- ) .1000000000
  PPVAL MONOE-01 ( H3O+ MEACOO- ) .1000000000
  PPVAL MONOE-01 ( H3O+ HCO3- ) .1000000000
  PPVAL MONOE-01 ( H3O+ OH- ) .1000000000
  PPVAL MONOE-01 ( H3O+ CO3-- ) .1000000000

STREAM 4
  SUBSTREAM MIXED TEMP=30. PRES=4.000000039 <psig> &
    MASS-FLOW=4000. <lb/hr>
  MASS-FRAC H2O 0.99999999438 / H3O+ 2.29E-009 / OH- &
    2.05E-009

STREAM 13
  SUBSTREAM MIXED TEMP=46.1220775 PRES=1.15114515
  MASS-FLOW H2O 1788.25229 / CO2 6437.92689 / N2 &
    24295.1313

STREAM 15
  SUBSTREAM MIXED TEMP=35.0464605 PRES=19.6959488 <psi> &
    MASS-FLOW=41.7848564 <kg/sec>
  MOLE-FRAC H2O 0.90824942 / CO2 6.8737E-007 / N2 &
    6.7018E-006 / MONOE-01 0.04106354 / MEA+ 0.02553813 / &
    H3O+ 0. / MEACOO- 0.02397746 / HCO3- 0.00076297 / &
    OH- 4.4679E-006 / CO3-- 0.00039661

STREAM 20
  SUBSTREAM MIXED TEMP=35.0464605 PRES=19.6959488 <psi> &
    MASS-FLOW=41.7848564 <kg/sec>
  MOLE-FRAC H2O 0.90824942 / CO2 6.8737E-007 / N2 &
    6.7018E-006 / MONOE-01 0.04106354 / MEA+ 0.02553813 / &
    H3O+ 0. / MEACOO- 0.02397746 / HCO3- 0.00076297 / &
    OH- 4.4679E-006 / CO3-- 0.00039661
```

```
STREAM 24
   SUBSTREAM MIXED TEMP=89. PRES=2.392
   MASS-FLOW H2O 105538.398 / CO2 159.667713 / N2  &
      0.58715253 / MONOE-01 2994.17622 / MEA+ 18210.8628 /  &
      H3O+ 0.00011379 / MEACOO- 25967.8089 / HCO3-  &
      2548.32392 / OH- 0.03788375 / CO3-- 61.295187

STREAM FLUEGAS
   SUBSTREAM MIXED TEMP=142. PRES=161.655436 <psi>  &
      MASS-FLOW=69000. <lb/hr>
   MOLE-FRAC H2O 0.03 / CO2 0.13999999 / N2 0.82999999

STREAM H2OMK
   SUBSTREAM MIXED TEMP=35. PRES=19.6959488 <psi>
   MASS-FLOW H2O 841.96

STREAM MEAMK
   SUBSTREAM MIXED TEMP=35. PRES=19.6959488 <psi>
   MASS-FLOW MONOE-01 1.3

STREAM XLEANOIL
   SUBSTREAM MIXED TEMP=35.0464605 PRES=19.6959488 <psi>  &
      MASS-FLOW=41.7848564 <kg/sec>
   MOLE-FRAC H2O 0.908249419 / CO2 6.87368E-007 / N2  &
      6.70184E-006 / MONOE-01 0.041063542 / MEA+ 0.025538131 / &
      H3O+ 0. / MEACOO- 0.023977461 / HCO3- 0.000762979 /  &
      OH- 4.46789E-006 / CO3-- 0.000396611

BLOCK B9 MIXER
   PARAM PRES=19.6959488 <psi> T-EST=35.

BLOCK B14 MIXER
   PARAM PRES=19.6959488 <psi> T-EST=35.0464605

BLOCK B13 FSPLIT
   FRAC 18 1.

BLOCK B2 HEATER
   PARAM TEMP=89. PRES=20. <psig>
   UTILITY UTILITY-ID=U-2

BLOCK B4 HEATER
   PARAM TEMP=30. PRES=1.
   UTILITY UTILITY-ID=U-1

BLOCK B8 HEATER
   PARAM TEMP=35. PRES=19.6959488 <psi>
```

```
   UTILITY UTILITY-ID=U-1

BLOCK B12 HEATER
   PARAM TEMP=30. PRES=1.

BLOCK B5 FLASH2
   PARAM TEMP=30. PRES=1.

BLOCK B15 FLASH2
   PARAM TEMP=30. PRES=1.

BLOCK SCRUBBER FLASH2
   PARAM TEMP=46.1220775 PRES=2. <psig>

BLOCK CROSSHX HEATX
   PARAM T-COLD=75. MIN-TAPP=5. U-OPTION=PHASE &
     F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
   FEEDS HOT=11 COLD=1
   PRODUCTS HOT=17 COLD=16
   FLASH-SPECS 17 NPHASE=1 PHASE=L FREE-WATER=NO

BLOCK ABSORBER RADFRAC
   PARAM NSTAGE=25
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS SCRUBGAS 25 ON-STAGE / XLEANOIL 1 ON-STAGE
   PRODUCTS ABSVENT 1 V / RICHOIL 25 L
   P-SPEC 1 0. <psig>
   COL-SPECS
   PACK-SIZE 1 1 4 RASCHIG VENDOR=RASCHIG PACK-MAT=METAL &
     PACK-SIZE="25-MM" HETP=3. <meter> P-UPDATE=NO

BLOCK B3 RADFRAC
   PARAM NSTAGE=11
   COL-CONFIG CONDENSER=NONE
   FEEDS 3 1 ON-STAGE / 10 1 ON-STAGE
   PRODUCTS 5 1 V / 6 11 L
   P-SPEC 1 1.73
   COL-SPECS MASS-RR=22.36063898
   UTILITIES REB-UTIL=U-2

BLOCK B10 RADFRAC
   PARAM NSTAGE=25
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   FEEDS 13 25 ON-STAGE / 15 1 ON-STAGE
   PRODUCTS 22 1 V / 23 25 L
   P-SPEC 1 0. <psig>
   COL-SPECS
```

```
BLOCK B11 RADFRAC
  PARAM NSTAGE=24
  COL-CONFIG CONDENSER=NONE
  FEEDS 24 1 ON-STAGE / 29 1 ON-STAGE
  PRODUCTS 25 1 V / 30 24 L
  P-SPEC 1 1.73
  COL-SPECS MASS-RR=22.360639

BLOCK B1 PUMP
  PARAM PRES=20. <psig>

BLOCK B6 PUMP
  PARAM PRES=2.392

BLOCK B7 PUMP
  PARAM PRES=19.6959488 <psi>

BLOCK B16 PUMP
  PARAM PRES=2.392

UTILITY U-1 GENERAL
  COST PRICE=0.01 <$/kg>
  PARAM UTILITY-TYPE=WATER TIN=30. TOUT=40. VFRAC=0.  &
    VFR-OUT=0. CALOPT=FLASH

UTILITY U-2 GENERAL
  COST PRICE=0.01 <$/kg>
  PARAM UTILITY-TYPE=STEAM PRES=150. <psig> PRES-OUT=150. <psig>
&
    VFRAC=1. VFR-OUT=0. CALOPT=FLASH

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW MASSFLOW

PROPERTY-REP NOPARAM-PLUS
;
;
;
;
;
```

Appendix F: Aspen Plus® Input Files for IL Process

Input Summary

ASPEN Plus® Input Files for MEA and Ionic Liquid Processes

IL Process:

```
;
;Input Summary created by Aspen Plus Rel. 23.0 at 11:49:06 Sat Feb 22, 2014
;Directory C:\Users\Administrator\Desktop\Diary GAMS\ORIGINAL_IL\211156\IL
Filename C:\Users\ADMINI~1\AppData\Local\Temp\~ap788f.tmp
;


DYNAMICS
   DYNAMICS RESULTS=ON

TITLE 'ionic liquid'

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C  &
      VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'  &
      MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
      MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l'  &
      PDROP=bar

DEF-STREAMS CONVEN ALL

SIM-OPTIONS OLD-DATABANK=YES

DESCRIPTION "
   General Simulation with Metric Units :
   C, bar, kg/hr, kmol/hr, Gcal/hr, cum/hr.

   Property Method: None

   Flow basis for input: Mole

   Stream report composition: Mole flow
   "

DATABANKS PURE22 / AQUEOUS / SOLIDS / INORGANIC / &
      NOASPENPCD

PROP-SOURCES PURE22 / AQUEOUS / SOLIDS / INORGANIC
```

```
COMPONENTS
  N2 N2 /
  O2 O2 /
  CO CO /
  CO2 CO2 /
  CH4 CH4 /
  H2O H2O /
  BMIMAC /
  BMIMCO2 /
  BMIM2CO2 /
  BMIM3CO2 /
  DICHL-01 CCL2F2

HENRY-COMPS HC-1 N2 O2 CO CO2 CH4

FLOWSHEET
  BLOCK B2 IN=5 37 OUT=7 8
  BLOCK B1 IN=3 OUT=1 2
  BLOCK B19 IN=35 OUT=36
  BLOCK B20 IN=36 OUT=37
  BLOCK B3 IN=6 OUT=3
  BLOCK B4 IN=9 8 OUT=4 6
  BLOCK B5 IN=2 OUT=9
  BLOCK B6 IN=4 OUT=10
  BLOCK B7 IN=10 12 OUT=11 13
  BLOCK B8 IN=13 OUT=14
  BLOCK B9 IN=14 OUT=15
  BLOCK B10 IN=15 OUT=16

PROPERTIES PR-BM
  PROPERTIES NRTL-RK

PROP-REPLACE PR-BM PR-BM
  PROP HLMX HLMX04

PROP-DATA IL
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kJ/kmol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST MW / TB / TC / PC / VC / OMEGA / ZC / &
    DHFORM
  PVAL BMIMAC 170.21 / 568.21 / 1673.15 / 29.14336 / 561 / &
    0.54919501 / 0.24646424 / -402310
  PVAL BMIMCO2 214.22 / 568.21 / 1673.15 / 29.14336 / &
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      655.255 / 0.54919501 / 0.24646424 / -795819
    PVAL BMIM2CO2 384.43 / 568.21 / 1673.15 / 29.14336 / &
      1216.255 / 0.54919501 / 0.24646424 / -1198129
    PVAL BMIM3CO2 554.64 / 568.21 / 1673.15 / 29.14336 / &
      1777.255 / 0.54919501 / 0.24646424 / -1600439

  PROP-DATA CPIG-1
    IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
      MOLE-HEAT-CA='J/kmol-K' HEAT-TRANS-C='kcal/hr-sqm-K' &
      PRESSURE=bar TEMPERATURE=K VOLUME=cum DELTA-T=C &
      HEAD=meter MOLE-DENSITY='kmol/cum' MASS-DENSITY='kg/cum' &
      MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg' HEAT=Gcal &
      MOLE-CONC='mol/l' PDROP=bar
    PROP-LIST CPIG
    PVAL BMIMAC 42972.1607 584.70684 -0.121380824 0 0 0 0 &
      1000 0 0 0
    PVAL BMIMCO2 82993.8012 683.179848 -0.340574471 0 0 0 0 &
      1000 0 0 0
    PVAL BMIM2CO2 1.49E+05 1226.00518 -0.611180301 0 0 0 0 &
      1000 0 0 0
    PVAL BMIM3CO2 2.15E+05 1768.83051 -0.88178613 0 0 0 0 &
      1000 0 0 0

  PROP-DATA DHVLDP-1
    IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K &
      VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
      MASS-DENSITY='kg/cum' MOLE-ENTHALP='J/kmol' &
      MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
      PDROP=bar
    PROP-LIST DHVLDP
    PVAL BMIMAC 55000000 0 0 0 0 0 1673.15
    PVAL BMIMCO2 69220962.34 0 0 0 0 0 1673.15
    PVAL BMIM2CO2 124220962.3 0 0 0 0 0 1673.15
    PVAL BMIM3CO2 179220962.3 0 0 0 0 0 1673.15

  PROP-DATA DNLDIP-1
    IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K &
      VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
      MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
      MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
      PDROP=bar
    PROP-LIST DNLDIP
    PVAL BMIMAC 0.372520301 0.220678391 1110.03716 0.528581257 &
      0 0 1000
    PVAL BMIMCO2 0.619120163 0.319086761 968.548727 0.613262615 &
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    0 0 1000
  PVAL BMIM2CO2 0.646694427 0.436693426 806.606681  &
    0.710224366 0 0 1000
  PVAL BMIM3CO2 0.256972399 0.330770016 952.277593  &
    0.623000575 0 0 1000

PROP-DATA KLDIP-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K  &
    THERMAL-COND='Watt/m-K' VOLUME=cum DELTA-T=C HEAD=meter
&
    MOLE-DENSITY='kmol/cum' MASS-DENSITY='kg/cum'  &
    MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg' HEAT=Gcal  &
    MOLE-CONC='mol/l' PDROP=bar
  PROP-LIST KLDIP
  PVAL BMIMAC 17307350 0 0 0 0 0 1673.15
  PVAL BMIMCO2 17307350 0 0 0 0 0 1673.15
  PVAL BMIM2CO2 17307350 0 0 0 0 0 1673.15
  PVAL BMIM3CO2 17307350 0 0 0 0 0 1673.15

PROP-DATA KVDIP-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K  &
    THERMAL-COND='Watt/m-K' VOLUME=cum DELTA-T=C HEAD=meter
&
    MOLE-DENSITY='kmol/cum' MASS-DENSITY='kg/cum'  &
    MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg' HEAT=Gcal  &
    MOLE-CONC='mol/l' PDROP=bar
  PROP-LIST KVDIP
  PVAL N2 3.31430000E-4 .7722000000 16.32300000 373.7200000  &
    0.0 0 1500
  PVAL O2 0.00044994 0.7456 56.699 0 0 0 1500
  PVAL CO 5.98820000E-4 .6863000000 57.13000000 501.9200000  &
    0.0 0 1500
  PVAL CO2 3.69 -0.3838 964 1860000 0 0 1500
  PVAL CH4 0.0000083983 1.4268 -49.6540 0 0 0 1500
  PVAL H2O 0.0000062041 1.3973 0 0 0 0 1500
  PVAL BMIMAC 0.1730735 0 0 0 0 0 1500
  PVAL BMIMCO2 0.1730735 0 0 0 0 0 1500
  PVAL BMIM2CO2 0.1730735 0 0 0 0 0 1500
  PVAL BMIM3CO2 0.1730735 0 0 0 0 0 1500

PROP-DATA MULDIP-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K  &
    VISCOSITY='N-sec/sqm' VOLUME=cum DELTA-T=C HEAD=meter  &
    MOLE-DENSITY='kmol/cum' MASS-DENSITY='kg/cum'  &
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      MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg' HEAT=Gcal  &
      MOLE-CONC='mol/l' PDROP=bar
   PROP-LIST MULDIP
   PVAL BMIMAC -328.819511 20301.9511 46.4267685 -7.05353998  &
      -0.060578654 0 1000
   PVAL BMIMCO2 -328.819511 20301.9511 46.4267685 -7.05353998  &
      -0.060578654 0 1000
   PVAL BMIM2CO2 -328.819511 20301.9511 46.4267685 -7.05353998  &
      -0.060578654 0 1000
   PVAL BMIM3CO2 -328.819511 20301.9511 46.4267685 -7.05353998  &
      -0.060578654 0 1000

PROP-DATA MUVDIP-1
   IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K  &
      VISCOSITY='N-sec/sqm' VOLUME=cum DELTA-T=C HEAD=meter  &
      MOLE-DENSITY='kmol/cum' MASS-DENSITY='kg/cum'  &
      MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg' HEAT=Gcal  &
      MOLE-CONC='mol/l' PDROP=bar
   PROP-LIST MUVDIP
   PVAL BMIMAC 0.000010 0 0 0 0 0 1500
   PVAL BMIMCO2 0.000010 0 0 0 0 0 1500
   PVAL BMIM2CO2 0.000010 0 0 0 0 0 1500
   PVAL BMIM3CO2 0.000010 0 0 0 0 0 1500

PROP-DATA PLXANT-1
   IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=Pa TEMPERATURE=K  &
      VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum'  &
      MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol'  &
      MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l'  &
      PDROP=bar
   PROP-LIST PLXANT
   PVAL BMIMAC 5.54919467 -5756.09503 -43.7150238 -2.78E-04  &
      0.518241563 4.73809692 -0.114237361 0 1000
   PVAL BMIMCO2 5.54919467 -5756.09503 -43.7150238 -2.78E-04  &
      0.518241563 4.73809692 -0.114237361 0 1000
   PVAL BMIM2CO2 5.54919467 -5756.09503 -43.7150238 -2.78E-04  &
      0.518241563 4.73809692 -0.114237361 0 1000
   PVAL BMIM3CO2 5.54919467 -5756.09503 -43.7150238 -2.78E-04  &
      0.518241563 4.73809692 -0.114237361 0 1000

PROP-DATA SIGDIP-1
   IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr'  &
      HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar  &
      SURFACE-TENS='N/m' TEMPERATURE=K VOLUME=cum DELTA-T=C
&
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    HEAD=meter MOLE-DENSITY='kmol/cum' MASS-DENSITY='kg/cum' &
    MOLE-ENTHALP='kcal/mol' MASS-ENTHALP='kcal/kg' HEAT=Gcal &
    MOLE-CONC='mol/l' PDROP=bar
  PROP-LIST SIGDIP
  PVAL BMIMAC .0272676789 -2.893649690 5.889672620 0.0 0.0 &
    0.0 1000.000000
  PVAL BMIMCO2 .0272676789 -2.893649690 5.889672620 0.0 0.0 &
    0.0 1000.000000
  PVAL BMIM2CO2 .0272676789 -2.893649690 5.889672620 0.0 0.0 &
    0.0 1000.000000
  PVAL BMIM3CO2 .0272676789 -2.893649690 5.889672620 0.0 0.0 &
    0.0 1000.000000

PROP-DATA HENRY-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST HENRY
  BPVAL N2 BMIMAC -212.8986616 9377.806300 33.61915830 0.0 &
    0.0 2000.000000 0.0
  BPVAL CO2 BMIMAC -953.8656576 -10000.00000 171.3430720 0.0 &
    0.0 2000.000000 0.0
  BPVAL N2 BMIMCO2 -212.8986616 9377.806300 33.61915830 0.0 &
    0.0 2000.000000 0.0
  BPVAL CO2 BMIMCO2 -953.8656576 -10000.00000 171.3430720 0.0 &
    0.0 2000.000000 0.0
  BPVAL N2 BMIM2CO2 -212.8986616 9377.806300 33.61915830 0.0 &
    0.0 2000.000000 0.0
  BPVAL CO2 BMIM2CO2 -953.8656576 -10000.00000 171.3430720 &
    0.0 0.0 2000.000000 0.0
  BPVAL N2 BMIM3CO2 -212.8986616 9377.806300 33.61915830 0.0 &
    0.0 2000.000000 0.0
  BPVAL CO2 BMIM3CO2 -953.8656576 -10000.00000 171.3430720 &
    0.0 0.0 2000.000000 0.0

PROP-DATA HENRY-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST HENRY
  BPVAL N2 H2O 164.9940745 -8432.770000 -21.55800000 &
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    -8.4362400E-3 -.1500000000 72.85000000 0.0
  BPVAL O2 H2O 144.4080745 -7775.060000 -18.39740000 &
    -9.4435400E-3 .8500000000 74.85000000 0.0
  BPVAL CO H2O 171.7750745 -8296.750000 -23.33720000 0.0 &
    -.1500000000 79.85000000 0.0
  BPVAL CO2 H2O 159.8650745 -8741.550000 -21.66900000 &
    1.10259000E-3 -.1500000000 79.85000000 0.0
  BPVAL CH4 H2O 183.7810745 -9111.670000 -25.03790000 &
    1.43434000E-4 1.850000000 79.85000000 0.0

PROP-DATA NRTL-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST NRTL
  BPVAL BMIMAC H2O 80 10000 0.338353607 0 0 0 1.26E-08 &
    1000
  BPVAL H2O BMIMAC 9.78912639 -3521.07339 0.338353607 0 0 0 &
    1.26E-08 1000
  BPVAL BMIMCO2 H2O 80 10000 0.338353607 0 0 0 1.26E-08 &
    1000
  BPVAL H2O BMIMCO2 9.78912639 -3521.07339 0.338353607 0 0 &
    0 1.26E-08 1000
  BPVAL BMIM2CO2 H2O 80 10000 0.338353607 0 0 0 1.26E-08 &
    1000
  BPVAL H2O BMIM2CO2 9.78912639 -3521.07339 0.338353607 0 0 &
    0 1.26E-08 1000
  BPVAL BMIM3CO2 H2O 80 10000 0.338353607 0 0 0 1.26E-08 &
    1000
  BPVAL H2O BMIM3CO2 9.78912639 -3521.07339 0.338353607 0 0 &
    0 1.26E-08 1000

PROP-DATA PRKBV-1
  IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
    HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=K &
    VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
    MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
    MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
    PDROP=bar
  PROP-LIST PRKBV
  BPVAL BMIMAC H2O 0 0 0 0 1000
  BPVAL H2O BMIMAC 0 0 0 0 1000
  BPVAL BMIMCO2 H2O 0 0 0 0 1000
  BPVAL H2O BMIMCO2 0 0 0 0 1000
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  BPVAL BMIM2CO2 H2O 0 0 0 0 1000
  BPVAL H2O BMIM2CO2 0 0 0 0 1000
  BPVAL BMIM3CO2 H2O 0 0 0 0 1000
  BPVAL H2O BMIM3CO2 0 0 0 0 1000

STREAM 5
  SUBSTREAM MIXED TEMP=-1.982417582 PRES=100. <psig>  &
    MASS-FLOW=47.9755475 <kg/sec>
  MOLE-FRAC N2 7.25363E-006 / O2 0. / CO 0. / CO2  &
    0.005926937 / CH4 0. / H2O 0.000790645 / BMIMAC  &
    0.738535827 / BMIMCO2 0.014595745 / BMIM2CO2  &
    0.091682921 / BMIM3CO2 0.148460672

STREAM 12
  SUBSTREAM MIXED TEMP=-30.4 VFRAC=0.252  &
    MASS-FLOW=28.6 <kg/sec>
  MASS-FRAC DICHL-01 1.

STREAM 35
  SUBSTREAM MIXED TEMP=142. PRES=101.32 <kPa>
  MOLE-FLOW N2 867.266 / CO2 146.26

BLOCK B3 HEATER
  PARAM TEMP=58.1341045 PRES=74.9373733 <psig>
  UTILITY UTILITY-ID=U-1

BLOCK B6 HEATER
  PARAM TEMP=45. PRES=100. <psig>
  UTILITY UTILITY-ID=U-2

BLOCK B9 HEATER
  PARAM TEMP=16. PRES=5.79

BLOCK B20 HEATER
  PARAM TEMP=39. PRES=100. <psig>
  UTILITY UTILITY-ID=U-2

BLOCK B4 HEATX
  PARAM DUTY=2441.357205 <kW> MIN-TAPP=5. U-OPTION=PHASE  &
    F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
  FEEDS HOT=9 COLD=8
  PRODUCTS HOT=4 COLD=6

BLOCK B7 HEATX
  PARAM T-HOT=-1.9824176 MIN-TAPP=5. U-OPTION=PHASE  &
    F-OPTION=CONSTANT CALC-METHOD=SHORTCUT
  FEEDS HOT=10 COLD=12
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   PRODUCTS HOT=11 COLD=13

BLOCK B2 RADFRAC
   PARAM NSTAGE=20 MAXOL=100
   COL-CONFIG CONDENSER=NONE REBOILER=NONE
   RATESEP-ENAB CALC-MODE=EQUILIBRIUM
   FEEDS 5 1 ON-STAGE / 37 20 ON-STAGE
   PRODUCTS 7 1 V / 8 20 L
   P-SPEC 1 74.9373733 <psig>
   COL-SPECS
   REAC-STAGES 1 20 R-1

BLOCK B1 RCSTR
   PARAM VOL=100. <cuft> TEMP=80.77858546 PRES=0. <psig>  &
     NPHASE=2
   PRODUCTS 1 V / 2 L
   BLOCK-OPTION FREE-WATER=NO
   REACTIONS RXN-IDS=R-2

BLOCK B5 PUMP
   PARAM PRES=100. <psig>

BLOCK B8 COMPR
   PARAM TYPE=ISENTROPIC PRES=5.79

BLOCK B19 COMPR
   PARAM TYPE=ISENTROPIC PRES=100. <psig>

BLOCK B10 VALVE
   PARAM P-OUT=0.98943169

UTILITY U-1 GENERAL
   COST PRICE=0.01 <$/kg>
   PARAM UTILITY-TYPE=STEAM PRES=125. <psig> PRES-OUT=125. <psig>
&
      VFRAC=1. VFR-OUT=0. CALOPT=FLASH

UTILITY U-2 GENERAL
   COST PRICE=0.01 <$/kg>
   PARAM UTILITY-TYPE=WATER TIN=30. TOUT=38. VFRAC=0.  &
     VFR-OUT=0. CALOPT=FLASH

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW

PROPERTY-REP PCES
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REACTIONS R-1 REAC-DIST
   REAC-DATA 1 KBASIS=MOLEFRAC
   REAC-DATA 2 KBASIS=MOLEFRAC
   REAC-DATA 3 KBASIS=MOLEFRAC
   K-STOIC 1 A=-6.5655 B=2743.9
   K-STOIC 2 A=7.6412 B=-1942.5
   K-STOIC 3 A=-0.7193 B=531.27
   STOIC 1 CO2 -1. / BMIMAC -1. / BMIMCO2 1.
   STOIC 2 BMIMCO2 -1. / BMIMAC -1. / BMIM2CO2 1.
   STOIC 3 BMIM2CO2 -1. / BMIMAC -1. / BMIM3CO2 1.

REACTIONS R-2 POWERLAW
   REAC-DATA 1 EQUIL KBASIS=MOLEFRAC
   REAC-DATA 2 EQUIL KBASIS=MOLEFRAC
   REAC-DATA 3 EQUIL KBASIS=MOLEFRAC
   K-STOIC 1 A=-6.5655 B=2743.9
   K-STOIC 2 A=7.6412 B=-1942.5
   K-STOIC 3 A=-0.7193 B=531.27
   STOIC 1 MIXED CO2 -1. / BMIMAC -1. / BMIMCO2 1.
   STOIC 2 MIXED BMIMCO2 -1. / BMIMAC -1. / BMIM2CO2 1.
   STOIC 3 MIXED BMIM2CO2 -1. / BMIMAC -1. / BMIM3CO2 1.
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;
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;
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CURRICULUM VITAE

Name: Mr. Koon Khonkaen

Date of Birth: April 20, 1990

Nationality: Thai

University Education:

2008-2011 Bachelor Degree of Engineering (Petrochemical and Polymeric Materials), Silpakorn University, Thailand.

Work Experience:

2011 Position: Production Engineer

Company name: Thai Manufacturing Company Limited

Proceeding:

1. Khonkaen, K.; Siemanond, K.; and Henni, A. (2014, April 22) Process Simulation of Carbon Dioxide Capture Using Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate. Proceeding of the 5th Research Symposium on Petrochemicals and Materials Technology and The 20th PPC Symposium on Petroleum, Petrochemicals, and Polymers, Bangkok, Thailand.
2. Khonkaen, K.; Siemanond, K.; and Henni, A. (2014, June 15-18) Process Simulation of Carbon Dioxide Capture Using Ionic Liquid 1-Ethyl-3-methylimidazolium Acetate. European Symposium on Computer Aided Process Engineering, Budapest, Hungary.