

CHAPTER IV

RESULTS OF CALCULATIONS

4.1 The Optimum Binary Interaction Parameters

The optimum binary interaction parameters predicted by both objective functions for each equation of state are given in Table 4.1 to Table 4.11. Tables 4.1 and 4.2 show the values of K_{ij} and the absolute average percent deviation (AAD) in bubble point pressures using five equations for systems containing methane, whereas Tables 4.3 and 4.4 are for systems containing ethane, Tables 4.5 and 4.6 are for systems containing propane, Tables 4.7 and 4.8 are for systems containing nitrogen and Tables 4.9 and 4.10 are for systems containing carbon dioxide. In those tables, "N" is the number of experimental data points used to evaluate the optimum K_{ij} , "Range of P" is the minimum and maximum pressure of the data set for the temperature (T) specified in the third column. In addition, the "Initial Range" is the first guess of K_{ij} value, which will be the same at all temperatures for the chosen binary system. In the study, "AAD(%)", the absolute average percent deviation in the predicted bubble point pressure is defined as

$$\%AAD = \frac{100}{N} \sum_{i=1}^N \frac{|P_i^{EXP} - P_i^{CAL}|}{P_i^{EXP}} \quad (4.1)$$

The deviation in the predicted vapor phase composition, DY and the deviation in predicted bubble point pressure, DP are shown in Appendix B as

$$DY = |y^{CAL} - y^{EXP}| \quad (4.2)$$

$$DP = |P^{CAL} - P^{EXP}| \quad (4.3)$$

y^{CAL} and y^{EXP} are the calculated and experimental vapor phase compositions.

Table 4.1 Binary interaction parameters and percent AAD for systems containing methane of five equations of state using the fugacity criterion

SYSTEM	Ref	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)	K _{ij}	AAD(%)						
Methane - Ethane	30	130.370	1.9053-3.3070	4	0.0111	0.7703	0.0000	2.2086	0.0028	1.4585	0.0069	1.0768	-0.0056	3.2666
	30	144.260	1.8577-6.6665	7	0.0042	0.7006	0.0069	0.9302	0.0042	1.0802	0.0069	0.7233	0.0056	0.5394
	30	158.150	1.7556-13.5412	10	0.0000	3.1899	0.0042	3.3078	0.0000	3.3774	0.0028	2.1412	0.0028	2.8165
	30	172.040	2.0958-23.1016	9	-0.0014	1.4581	0.0042	1.4113	-0.0014	1.3593	0.0014	1.3021	0.0056	1.1043
	30	186.110	2.4973-35.6561	8	-0.0042	0.7849	0.0028	1.0862	-0.0042	0.9280	-0.0028	0.9085	0.0056	0.9739
	30	189.650	2.4360-41.8483	10	-0.0069	0.9479	0.0000	2.8073	-0.0069	3.4210	-0.0056	4.0630	0.0028	3.0678
	30	190.940	2.6878-45.4547	10	-0.0056	2.7804	0.0014	5.6668	-0.0056	3.5423	-0.0056	10.3015	0.0042	7.5545
	30	192.380	2.6538-40.8276	8	-0.0097	0.8965	-0.0028	1.0041	-0.0097	1.1063	-0.0097	0.9351	0.0014	0.8632
	30	199.920	3.0621-40.8276	8	-0.0139	1.4047	-0.0069	1.4690	-0.0139	1.5929	-0.0153	1.3140	-0.0028	1.2609
	31	260.000	17.8000-55.1600	10	0.0083	1.1303	0.0139	0.9631	0.0069	0.8589	-0.0097	0.5761	0.0167	0.6914
	31	270.000	22.5300-50.2600	9	0.0222	1.1074	0.0250	1.0148	0.0194	0.7801	-0.0014	0.5988	0.0250	0.6077
<i>Initial Range : [-0.05, 0.15]</i>	31	280.000	28.5000-46.5000	7	0.0333	2.1364	0.0347	5.9708	0.0278	1.6069	0.0056	5.2859	0.0361	1.6699
Methane - Propane	32	144.260	2.1094-7.3490	6	0.0156	2.4075	-0.0010	6.2612	0.0010	3.4249	0.0167	2.4602	-0.0073	9.1607
	32	158.150	1.7011-13.7113	8	0.0271	4.4945	0.0177	2.1680	0.0156	1.9540	0.0260	2.9178	0.0177	2.1677
	32	172.040	2.0958-23.2717	8	0.0146	2.1622	0.0198	1.6795	0.0115	1.7225	0.0167	1.7919	0.0240	1.4740
	32	187.540	2.7699-39.8750	9	0.0125	1.4209	0.0188	1.3608	0.0094	1.4251	0.0135	1.4132	0.0250	1.4623
	32	192.300	2.0414-39.1264	9	0.0052	1.3529	0.0135	1.2676	0.0031	1.1524	0.0063	1.3212	0.0168	1.1756
	32	195.200	2.0754-44.2299	11	0.0094	1.4824	0.0167	1.3722	0.0063	1.2400	0.0094	1.4944	0.0229	1.3669
<i>Initial Range : [-0.05, 0.10]</i>	32	213.710	1.8713-61.2414	11	0.0062	1.5100	0.0135	1.5216	0.0021	1.1379	0.0031	1.9452	0.0219	1.7850
Methane - n-Butane	33	166.493	1.3609-19.2570	8	0.0229	2.0233	0.0292	1.9314	0.0188	1.9244	0.0229	1.7292	0.0271	1.6589
	33	177.604	1.3609-29.4906	8	0.0167	1.4487	0.0240	1.2953	0.0125	1.3040	0.0167	1.2608	0.0250	1.1607
	33	185.938	1.3609-37.3573	9	0.0229	3.3316	0.0302	3.1951	0.0177	2.8752	0.0229	3.3181	0.0312	2.9143
	33	194.104	1.3609-46.0671	10	0.0104	2.7861	0.0188	2.7074	0.0052	4.6728	0.0094	2.8612	0.0219	2.7121
	34	199.893	13.6160-51.0345	7	0.0094	2.5609	0.0177	2.3946	0.0052	2.1648	0.0083	2.8356	0.0219	2.4807
	33	210.938	1.3609-54.3007	9	0.0031	1.9298	0.0125	1.9793	-0.0021	1.7211	0.0010	2.1699	0.0188	2.0396
	33	227.580	3.4000-81.4400	8	0.0104	4.2508	0.0198	4.5880	0.0042	3.6803	0.0042	5.0568	0.0271	4.6728
	33	255.380	1.3600-108.6600	8	0.0188	4.1542	0.0323	5.0100	0.0135	3.7686	-0.0021	4.8308	0.0333	4.7360
	33	283.160	3.4703-95.2644	9	0.0125	1.4090	0.0208	1.4221	0.0042	1.7252	-0.0187	1.0762	0.0281	1.1573
Methane - Isobutane <i>Initial Range : [-0.05, 0.15]</i>	35	310.938	5.4437-108.8736	18	0.0278	0.6191	0.0347	1.2807	0.0167	0.6589	-0.0222	1.1800	0.0361	1.5108
	35	344.271	13.6092-95.2644	13	0.0542	0.4729	0.0569	0.7988	0.0375	0.2616	-0.0250	1.1112	0.0472	1.8809

Table 4.1 (Continued)

SYSTEM	Ref	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)	K _{ij}	AAD(%)	K _{ij}	AAD(%)	K _{ij}	AAD(%)	K _{ij}	AAD(%)
Methane - n-Pentane	36	178.221	1.3677–20.4274	6	0.0292	2.2482	0.0361	2.2995	0.0208	2.3676	0.0292	2.2766	0.0333	2.3744
	36	192.638	6.8182–40.8276	4	0.0208	5.2713	0.0292	5.0542	0.0125	5.5730	0.0208	5.1087	0.0292	5.3575
	36	194.182	6.8114–40.8276	4	0.0125	5.5515	0.0194	5.7054	0.0028	6.0337	0.0111	5.6279	0.0208	5.7305
	36	198.871	3.4159–40.8276	5	0.0056	5.9808	0.0139	5.9563	-0.0042	6.1826	0.0042	5.9560	0.0167	5.9493
	36	223.932	6.8182–81.6552	7	-0.0194	10.0068	0.0042	7.8231	-0.0278	10.2422	-0.0250	9.7206	-0.0042	10.1484
	36	248.349	6.8182–112.4828	10	0.0042	5.3859	0.0236	3.8556	-0.0014	4.4458	-0.0111	5.8735	0.0208	5.8284
	36	273.171	13.6228–136.0920	10	0.0181	7.3611	0.0403	5.0619	0.0153	6.3087	-0.0097	7.9441	0.0222	10.6723
	37	377.804	68.1140–136.0240	10	0.0417	1.1313	0.0542	1.2051	0.0236	0.9088	-0.0819	1.5345	0.0278	2.6597
Methane - Isopentane	37	344.271	34.1591–149.0686	8	0.0139	2.1625	0.0319	1.6031	0.0056	2.0450	-0.0639	1.4497	0.0222	2.1864
Initial Range : [-0.10,0.10]	37	377.804	33.9550–129.2194	7	0.0444	1.9362	0.0472	2.5901	0.0181	2.4929	-0.0722	2.0464	0.0319	1.6317
Methane - Neopentane	37	344.271	21.0943–118.9444	9	0.0431	1.6612	0.0500	2.2254	0.0236	2.2649	-0.0319	1.8226	0.0306	2.0420
Initial Range : [-0.10,0.10]	37	377.804	20.9582–85.1255	5	0.0847	3.1804	0.0881	4.2561	0.0825	3.6826	-0.0222	3.6264	0.0681	3.2503
Methane - n-Hexane	36	190.510	1.3609–33.9958	5	0.0444	1.9977	0.0507	2.0358	0.0326	1.8205	0.0417	2.0297	0.0458	2.0254
	36	193.160	1.3677–34.0298	5	0.0417	3.2920	0.0479	3.1143	0.0271	3.7387	0.0382	3.0570	0.0438	3.1320
	36	198.080	1.3541–40.8276	10	0.0451	1.2781	0.0507	1.2992	0.0306	1.2715	0.0417	1.2836	0.0479	1.2328
	36	210.160	1.3745–40.8276	9	0.0528	1.3224	0.0590	1.4517	0.0375	1.2543	0.0479	1.3840	0.0576	1.3831
	36	223.160	1.3745–68.0460	11	0.0444	2.7174	0.0507	2.5380	0.0289	2.7487	0.0375	2.7290	0.0521	2.5969
Initial Range : [0.00,0.10]	36	248.150	1.3677–68.0460	11	0.0479	2.2843	0.0576	2.7658	0.0299	2.0101	0.0361	2.3541	0.0604	2.3136
	36	273.170	1.7080–108.8796	13	0.0417	1.1852	0.0514	1.6182	0.0222	0.9754	0.0194	1.2889	0.0569	1.1369

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Table 4.2 Binary interaction parameters and percent AAD for systems containing methane of five equations of state using the bubble point pressure criterion

SYSTEM	Ref.	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Methane - Ethane	30	130.370	1.9053–3.3070	4	0.0111	0.7703	0.0083	1.7811	0.0089	1.3605	0.0097	1.0092	0.0083	0.8245
	30	144.260	1.8577–6.6685	7	0.0042	0.7006	0.0056	0.6271	0.0028	0.7367	0.0056	0.4649	0.0042	0.6482
	30	158.150	1.7556–19.5412	10	-0.0089	2.2919	-0.0028	2.3121	-0.0083	2.2438	-0.0056	2.1340	-0.0028	2.3973
	30	172.040	2.0958–23.1016	9	-0.0042	1.2603	0.0000	1.0973	-0.0042	1.1561	-0.0028	0.9869	0.0028	0.9490
	30	186.110	2.4973–35.6581	8	-0.0042	0.7849	0.0014	0.9778	-0.0042	0.9280	-0.0042	0.9133	0.0042	0.9421
	30	189.650	2.4360–41.8483	10	-0.0097	1.2949	0.0000	1.0623	-0.0208	3.7627	-0.0028	0.0566	-0.0097	5.0306
	30	190.940	2.6878–45.4547	10	-0.0028	3.8310	0.0264	7.0160	0.0014	3.7488	-0.0319	8.4028	0.0153	4.9629
	30	192.390	2.6638–40.8276	8	-0.0089	0.7879	-0.0028	1.0041	-0.0083	0.9912	-0.0083	0.8456	0.0014	0.8632
	30	199.920	3.0821–40.8276	8	-0.0083	0.9461	-0.0028	1.3087	-0.0083	1.2718	-0.0097	1.0256	0.0014	0.9224
	31	260.000	17.8000–55.1800	10	0.0028	0.9498	0.0083	0.6359	0.0042	0.7528	-0.0139	0.3665	0.0111	0.0904
	31	270.000	22.5300–50.2600	9	0.0139	0.9210	0.0167	0.6156	0.0139	0.6657	-0.0056	0.4663	0.0194	0.3020
<i>Initial Range : [-0.05, 0.15]</i>	31	280.000	28.5000–46.5000	7	0.0389	2.4575	0.0097	0.8624	0.0089	0.8293	-0.0167	0.7433	0.0125	0.5700
	32	144.260	2.1094–7.3490	6	0.0115	2.6210	0.0146	2.6365	0.0083	2.6334	0.0125	2.7275	0.0146	3.1218
	32	158.150	1.7011–13.7113	8	0.0167	1.8367	0.0219	1.7905	0.0135	1.8258	0.0186	1.5303	0.0229	1.3093
	32	172.040	2.0958–23.2717	8	0.0115	1.6796	0.0177	1.2619	0.0094	1.3097	0.0135	1.2097	0.0208	0.7349
	32	187.540	2.7899–39.8750	9	0.0094	1.3562	0.0177	1.3287	0.0073	1.3828	0.0104	1.3498	0.0219	1.3218
	32	192.300	2.0414–39.1264	9	0.0063	1.3235	0.0135	1.2676	0.0042	1.2459	0.0073	1.3833	0.0198	1.2702
	32	195.200	2.0754–44.2299	11	0.0083	1.5263	0.0156	1.3200	0.0063	1.2400	0.0083	1.5610	0.0219	1.3256
	32	213.710	1.8713–61.2414	11	0.0052	1.5100	0.0125	1.4707	0.0021	1.1379	0.0010	1.9450	0.0198	1.8331
<i>Initial Range : [-0.05, 0.10]</i>	33	166.493	1.3609–19.2570	8	0.0198	1.8273	0.0260	1.5549	0.0156	1.5230	0.0198	1.5389	0.0250	1.5461
	33	177.604	1.3609–29.4906	8	0.0156	1.5292	0.0229	1.1771	0.0115	1.0889	0.0167	1.2608	0.0240	0.9514
	33	185.938	1.3609–37.3573	9	0.0188	2.7503	0.0260	2.5158	0.0135	2.2348	0.0177	2.5954	0.0281	2.4766
	33	194.104	1.3609–46.0571	10	0.0083	2.8254	0.0167	2.5510	0.0031	2.2051	0.0073	2.9933	0.0198	2.6675
	34	199.893	13.6160–51.0345	7	0.0073	2.6807	0.0156	2.5219	0.0031	2.1879	0.0052	2.9200	0.0198	2.6062
	33	210.938	1.3609–54.3007	9	0.0031	1.9298	0.0115	1.9638	-0.0031	1.6353	-0.0010	2.1537	0.0177	1.9927
	33	227.560	3.4000–61.4400	8	0.0052	4.0906	0.0135	4.3663	-0.0010	3.3996	-0.0031	4.9462	0.0208	4.5713
	33	265.360	1.3600–108.6600	8	0.0125	3.7569	0.0198	3.9754	0.0042	3.0802	-0.0052	4.8396	0.0292	4.7539
	33	283.160	3.4703–95.2644	9	0.0104	1.5359	0.0177	1.3422	0.0000	1.7761	-0.0208	1.0455	0.0292	1.0668
Methane – Isobutane	35	310.938	5.4437–108.8736	18	0.0250	0.4701	0.0278	0.3886	0.0139	0.3354	-0.0264	1.0780	0.0347	1.5337
	35	344.271	13.6092–95.2644	13	0.0514	0.5169	0.0514	0.1981	0.0361	0.1929	-0.0278	1.1576	0.0486	1.8657

Table 4.2 (Continued)

SYSTEM	Ref.	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS			
					K _{ij}	AAD(%)	K _{ij}	AAD(%)	K _{ij}	AAD(%)	K _{ij}	AAD(%)	K _{ij}	AAD(%)		
Methane - n-Pentane	36	178.221	1.3677–20.4274	6	0.0319	2.7690	0.0375	2.5929	0.0236	2.8068	0.0306	2.4382	0.0361	2.7023		
	36	192.638	6.8182–40.8276	4	0.0208	5.2713	0.0278	5.3869	0.0125	5.5730	0.0208	5.1087	0.0292	5.3575		
	36	194.182	6.8114–40.8276	4	0.0181	6.0824	0.0264	6.1127	0.0097	6.5910	0.0181	6.0904	0.0278	6.1522		
	36	199.871	3.4159–40.8276	5	0.0111	6.2964	0.0194	6.2322	0.0028	6.8499	0.0111	6.4458	0.0222	6.3811		
	36	223.932	6.8182–81.6552	7	0.0000	7.5682	0.0063	7.2326	-0.0111	8.1634	-0.0056	7.2302	0.0153	7.5467		
	36	248.349	6.8182–112.4828	10	0.0153	3.8543	0.0222	3.6329	0.0028	3.9965	0.0028	3.8846	0.0333	3.8437		
	36	273.171	13.6228–136.0920	10	0.0292	5.8254	0.0361	5.3189	0.0139	6.3749	0.0069	5.5010	0.0486	5.5420		
<i>Initial Range : [-0.10,0.10]</i>					37	377.604	68.1140–136.0240	10	0.0472	0.6918	0.0472	0.6252	0.0194	0.7796	-0.0736	1.0226
Methane - Isopentane	37	344.271	34.1591–149.0688	8	0.0250	1.2755	0.0292	1.5836	0.0056	2.0450	-0.0569	1.1047	0.0319	1.1302		
	37	377.604	33.9550–129.2194	7	0.0369	1.7013	0.0417	2.3949	0.0153	2.4217	-0.0633	1.5528	0.0306	1.6639		
Methane - Neopentane	37	344.271	21.0943–118.9444	9	0.0375	1.8886	0.0403	2.1927	0.0194	2.3524	-0.0417	1.7297	0.0306	2.0420		
	37	377.604	20.9582–85.1255	5	0.0569	2.5151	0.0514	2.6931	0.0308	2.6929	-0.0583	2.1656	0.0369	1.7322		
Methane - n-Hexane	36	190.510	1.3609–33.9958	5	0.0472	2.3949	0.0528	2.3052	0.0340	2.3095	0.0438	2.3410	0.0479	2.3147		
	36	193.160	1.3677–34.0298	5	0.0451	2.8770	0.0514	2.8114	0.0319	3.1772	0.0424	2.8628	0.0472	2.8547		
	36	198.060	1.3541–40.8276	10	0.0444	1.3637	0.0507	1.2992	0.0308	1.2715	0.0410	1.3695	0.0472	1.3016		
	36	210.160	1.3745–40.8276	9	0.0514	1.5288	0.0576	1.6134	0.0361	1.4900	0.0465	1.6481	0.0563	1.5561		
	36	223.160	1.3745–68.0460	11	0.0431	3.0004	0.0500	2.6630	0.0271	3.1953	0.0368	2.9091	0.0507	2.9160		
	36	248.160	1.3677–68.0460	11	0.0465	2.4218	0.0528	2.8910	0.0271	2.0761	0.0340	2.5607	0.0576	2.5406		
	36	273.170	1.7080–108.8736	13	0.0431	1.0844	0.0486	1.3852	0.0208	0.8972	0.0215	1.1107	0.0569	1.1369		

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Table 4.3 Binary interaction parameters and percent AAD for systems containing ethane of five equations of state using the fugacity criterion

SYSTEM	Ref	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Ethane - Propane	39	195.000	0.2981–1.5623	15	0.0125	3.3166	0.0063	2.8822	0.0094	3.0490	0.0104	3.0698	0.0094	3.0678
	39	210.000	0.5073–2.8285	18	0.0083	1.6382	0.0063	2.2079	0.0073	2.0787	0.0083	2.0780	0.0094	1.8019
	39	225.000	0.7718–3.5529	18	0.0052	1.9117	0.0063	2.5104	0.0052	2.1215	0.0063	2.0131	0.0083	1.9896
	39	235.000	2.0183–7.1345	18	0.0021	3.1253	0.0010	2.7319	0.0000	2.6692	0.0010	2.4320	0.0042	2.2149
	39	245.000	2.2897–6.5295	18	0.0021	2.1638	0.0042	2.7818	0.0021	2.2218	0.0042	2.4623	0.0063	2.1606
	39	255.000	3.5885–9.2642	18	-0.0052	1.0014	-0.0021	1.3144	-0.0042	1.0254	-0.0031	0.9418	0.0000	0.8149
	39	270.000	4.8951–14.1683	18	0.0063	4.0116	0.0083	3.6965	0.0073	3.8631	0.0083	3.8089	0.0104	3.3912
Ethane - n-Butane	40	338.716	34.9756–47.7002	4	0.0278	1.5591	0.0308	1.5768	0.0264	1.5890	0.0188	1.3069	0.0278	1.4328
	40	366.493	34.6354–47.0198	6	0.0486	2.1003	0.0479	2.4000	0.0431	2.0329	0.0313	1.2402	0.0438	1.9958
Ethane - Isobutane	41	311.271	10.5471–39.8069	7	-0.0219	0.4554	-0.0177	0.4378	-0.0219	0.4552	-0.0229	0.4637	-0.0156	0.4416
<i>Initial Range : [-0.05, 0.10]</i>														

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Table 4.4 Binary interaction parameters and percent AAD for systems containing ethane of five equations of state using the bubble point pressure criterion

SYSTEM	Ref.	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Ethane - Propane	39	195.000	0.2961-1.5623	15	0.0125	3.3166	0.0063	2.8822	0.0094	3.0900	0.0094	3.0357	0.0104	3.0865
	39	210.000	0.5073-2.8285	18	0.0052	1.1720	0.0010	1.3240	0.0031	1.1930	0.0031	1.1826	0.0052	1.1484
	39	225.000	0.7718-3.5529	18	0.0010	1.6037	-0.0010	1.0967	-0.0010	1.3558	0.0000	1.1962	0.0031	1.0935
	39	235.000	2.0183-7.1345	18	-0.0073	2.1518	-0.0073	1.8705	-0.0063	1.9267	-0.0063	1.7270	-0.0031	1.4253
	39	245.000	2.2897-6.5295	18	-0.0052	0.5365	-0.0052	0.3221	-0.0052	0.4364	-0.0042	0.3747	-0.0010	0.4074
	39	255.000	3.5885-9.2642	18	-0.0083	0.4237	-0.0063	0.2919	-0.0073	0.3565	-0.0063	0.2859	-0.0031	0.2797
	39	270.000	4.6951-14.1683	18	-0.0125	0.2910	-0.0083	0.2806	-0.0104	0.2798	-0.0094	0.2479	-0.0042	0.4225
Ethane - n-Butane	40	338.718	34.9758-47.7002	4	0.0285	1.5779	0.0278	1.4971	0.0250	1.5488	0.0215	1.3806	0.0271	1.3969
	40	366.493	34.6354-47.0198	6	0.0354	1.0871	0.0326	1.0279	0.0333	1.1658	0.0257	0.9407	0.0326	0.9742
Ethane - Isobutane	41	311.271	10.5471-39.8069	7	-0.0219	0.4554	-0.0177	0.4978	-0.0208	0.3911	-0.0208	0.4885	-0.0146	0.4018

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Table 4.5 Binary interaction parameters and percent AAD for systems containing propane of five equations of state using the fugacity criterion

SYSTEM	Ref	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Propane - Propylene	42	230.000	0.9968–1.2139	9	0.0156	1.5066	0.0125	0.4737	0.0146	0.8256	0.0135	0.2434		
	42	240.000	1.5199–1.8357	9	0.0146	1.2395	0.0125	0.5436	0.0135	0.9957	0.0125	0.3698		
	42	250.000	2.2403–2.6748	9	0.0125	1.0076	0.0115	0.5349	0.0125	0.9134	0.0115	0.4197		
	42	260.000	3.1779–3.7789	9	0.0115	0.5837	0.0104	0.5618	0.0115	0.7688	0.0104	0.4245		
	42	270.000	4.3918–5.1912	9	0.0094	0.3678	0.0094	0.5523	0.0104	0.6181	0.0094	0.4160		
	42	280.000	5.9215–6.9677	9	0.0083	0.1729	0.0083	0.5031	0.0094	0.4566	0.0094	0.2063		
	42	290.000	7.8164–9.1488	9	0.0063	0.1498	0.0073	0.3898	0.0083	0.3004	0.0083	0.1255		
	42	300.000	10.1258–11.7937	9	0.0052	0.3579	0.0073	0.1347	0.0073	0.1834	0.0073	0.0718		
	42	310.000	12.8991–14.9716	9	0.0042	0.5283	0.0063	0.0987	0.0063	0.0974	0.0063	0.0249		
	42	320.000	16.1855–18.7318	9	0.0031	0.6113	0.0052	0.0750	0.0052	0.0703	0.0052	0.0622		
	42	330.000	20.0543–23.1335	9	0.0031	0.7485	0.0042	0.1085	0.0042	0.0604	0.0042	0.1052		
	42	340.000	24.5645–28.2556	9	0.0021	0.6560	0.0031	0.1498	0.0042	0.1415	0.0042	0.2617		
<i>Initial Range : [-0.05, 0.10]</i>														
Propane - Isopentane	43	273.160	0.5000–4.0000	8	0.0042	1.8750	0.0031	1.7890	0.0031	1.8784	0.0042	1.7965	0.0052	1.9228
	43	298.160	1.5000–7.0000	7	-0.0010	2.7875	0.0010	2.5659	-0.0010	2.9822	0.0010	2.6238	0.0021	2.9201
	43	348.160	5.0000–25.0000	8	0.0063	1.5283	0.0083	1.8621	0.0083	1.9840	0.0073	1.8968	0.0094	1.9950
	43	398.160	15.0000–35.0000	6	0.0312	1.2647	0.0312	5.1707	0.0292	0.9696	0.0281	0.8514	0.0312	1.0879

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Table 4.6 Binary interaction parameters and percent AAD for systems containing propane of five equations of state using the bubble point pressure criterion

SYSTEM	Ref.	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Propane - Propylene	42	230.000	0.9968–1.2139	9	0.0208	0.6106	0.0135	0.4846	0.0177	0.5631	0.0135	0.2434		
	42	240.000	1.5199–1.6357	9	0.0198	0.5468	0.0135	0.4642	0.0177	0.5357	0.0135	0.2269		
	42	250.000	2.2403–2.6746	9	0.0167	0.4095	0.0135	0.3436	0.0167	0.4343	0.0135	0.2130		
	42	260.000	3.1779–3.7789	9	0.0135	0.2868	0.0125	0.3018	0.0146	0.3555	0.0125	0.1753		
	42	270.000	4.3918–5.1912	9	0.0115	0.2520	0.0115	0.2610	0.0135	0.3149	0.0115	0.1352		
	42	280.000	5.9215–6.9877	9	0.0083	0.1729	0.0104	0.2111	0.0115	0.2290	0.0104	0.1283		
	42	290.000	7.8164–9.1486	9	0.0052	0.1647	0.0094	0.1756	0.0094	0.1752	0.0094	0.1193		
	42	300.000	10.1258–11.7937	9	0.0031	0.1504	0.0063	0.1532	0.0083	0.1282	0.0073	0.0718		
	42	310.000	12.8991–14.9716	9	0.0010	0.1930	0.0063	0.0987	0.0083	0.0974	0.0063	0.0249		
	42	320.000	16.1855–18.7318	9	-0.0010	0.2458	0.0052	0.0750	0.0052	0.0703	0.0052	0.0622		
<i>Initial Range : [-0.05, 0.10]</i>	42	330.000	20.0643–23.1335	9	-0.0021	0.2666	0.0031	0.0901	0.0042	0.0604	0.0031	0.0906		
	42	340.000	24.5645–28.2558	9	-0.0021	0.2474	0.0021	0.0996	0.0031	0.0680	0.0021	0.1053		
Propane - Isopentane	43	273.160	0.5000–4.0000	8	0.0073	1.7605	0.0063	1.5197	0.0052	1.2590	0.0063	1.5983	0.0073	1.2960
	43	298.160	1.5000–7.0000	7	0.0073	0.1880	0.0063	0.3397	0.0073	0.3382	0.0083	0.3633	0.0104	0.5711
	43	348.160	5.0000–25.0000	8	0.0052	1.8494	0.0094	1.7334	0.0073	1.8376	0.0083	1.7753	0.0104	1.8666
	43	398.160	15.0000–35.0000	6	0.0240	0.8688	0.0260	0.6444	0.0240	0.6300	0.0240	0.5665	0.0250	0.5260

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Table 4.7 Binary interaction parameters and percent AAD for systems containing nitrogen of five equations of state using the fugacity criterion

SYSTEM	Ref	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Nitrogen - Methane	44	113.716	8.24–57.48	8	0.0319	0.8889	0.0368	0.4860	0.0347	0.7738	0.0326	0.7715	0.0521	0.6343
	44	122.049	2.7559–25.8575	10	0.0278	0.9691	0.0326	3.6830	0.0308	0.6779	0.0285	0.7108	0.0493	0.8997
	44	127.604	3.4840–28.3752	7	0.0292	0.9787	0.0340	1.1373	0.0326	1.3532	0.0292	1.0090	0.0507	1.1476
	44	138.468	6.8216–33.8869	7	0.0292	0.7808	0.0340	1.4163	0.0333	1.8749	0.0285	0.8389	0.0528	1.1049
	44	149.827	12.1802–33.8828	6	0.0250	0.5449	0.0292	0.3685	0.0292	0.7713	0.0208	0.6250	0.0479	0.4964
	44	160.938	17.0115–40.6915	8	0.0375	1.3498	0.0403	1.6041	0.0424	1.9544	0.0299	0.8055	0.0604	1.2583
	44	172.049	25.2110–40.6915	6	0.0479	0.9646	0.0479	0.8862	0.0521	1.3318	0.0354	0.3933	0.0681	0.4103
<i>Initial Range : [0.00,0.20]</i>														
Nitrogen - Ethane	45	138.716	3.4840–34.0230	7	0.0500	3.9847	0.0625	4.5093	0.0542	3.9862	0.0521	3.9520	0.0771	4.7925
	45	149.827	3.4023–40.8956	8	0.0479	3.4889	0.0604	3.9930	0.0521	3.5001	0.0479	3.4492	0.0813	4.3290
	45	172.049	3.5724–67.9099	8	0.0375	3.8410	0.0500	4.3677	0.0417	3.9121	0.0292	3.8756	0.0771	4.7039
	45	194.271	3.4703–98.2851	9	0.0364	4.0797	0.0479	4.6317	0.0398	4.0702	0.0148	4.0274	0.0833	5.3979
	31	260.000	18.1000–93.8000	8	0.0604	2.1142	0.0667	2.4714	0.0583	1.9992	-0.0500	1.9175	0.1042	2.6017
	31	280.000	29.5000–80.9000	14	0.1021	2.2835	0.1000	1.9248	0.0917	1.9179	-0.0521	2.1091	0.1271	2.0028
	31	280.000	29.5000–80.9000	14	0.1021	2.2835	0.1000	1.9248	0.0917	1.9179	-0.0521	2.1091	0.1271	2.0028
Nitrogen - Carbon dioxide	46	220.000	14.8927–136.1559	8	-0.0233	2.9208	-0.0024	4.0155	-0.0233	2.9387	-0.0719	2.8197	0.0497	4.7297
	46	240.000	20.7254–142.8275	14	-0.0377	2.7419	-0.0111	3.4345	-0.0337	2.7158	-0.1118	2.9458	0.0340	5.0751
	47	270.000	39.0000–95.0000	18	-0.0042	0.6937	0.0080	1.0316	-0.0148	0.8612	-0.1431	0.8916	0.0740	1.4829
<i>Initial Range : [-0.10,0.20]</i>														

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Table 4.8 Binary interaction parameters and percent AAD for systems containing nitrogen of five equations of state using the bubble point pressure criterion

SYSTEM	Ref.	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Nitrogen - Methane	44	113.716	8.24–57.48	8	0.0340	0.7325	0.0361	0.4319	0.0340	0.7502	0.0333	0.6993	0.0521	0.6343
	44	122.049	2.7559–25.8575	10	0.0333	0.5629	0.0333	0.6202	0.0308	0.6779	0.0333	0.6045	0.0521	0.6755
	44	127.804	3.4840–28.3752	7	0.0278	0.9575	0.0299	0.9154	0.0271	0.9501	0.0271	0.9789	0.0486	1.0980
	44	136.468	6.8216–33.8889	7	0.0257	0.4579	0.0278	0.4740	0.0257	0.5940	0.0243	0.5198	0.0479	0.9002
	44	149.827	12.1802–33.8828	6	0.0271	0.4056	0.0292	0.3683	0.0278	0.7598	0.0250	0.1241	0.0493	0.3835
	44	160.838	17.0115–40.6915	8	0.0292	0.8189	0.0299	0.6703	0.0299	1.0850	0.0250	0.4778	0.0507	0.2199
	44	172.049	25.2110–40.6915	6	0.0382	0.6922	0.0382	0.5380	0.0375	0.8701	0.0340	0.3825	0.0625	0.2883
	<i>Initial Range : [0.00,0.20]</i>													
Nitrogen - Ethane	45	138.716	3.4840–34.0230	7	0.0468	4.3813	0.0583	4.8510	0.0521	3.9984	0.0479	4.1905	0.0750	4.7703
	45	149.827	3.4023–40.8956	8	0.0438	3.8429	0.0583	4.1813	0.0500	3.6823	0.0498	3.7672	0.0771	4.5001
	45	172.049	3.5724–67.9099	8	0.0375	3.8410	0.0500	4.3877	0.0417	3.9121	0.0313	3.5783	0.0792	4.8061
	45	194.271	3.4703–96.2651	9	0.0354	4.0797	0.0417	4.9975	0.0375	4.1283	0.0125	4.0909	0.0792	5.4197
	31	260.000	18.1000–98.9000	8	0.0417	1.3223	0.0500	1.2142	0.0386	1.2503	-0.0708	1.4780	0.0833	2.1380
	31	280.000	29.5000–80.9000	14	0.0667	1.2258	0.0750	0.8197	0.0604	1.1315	-0.0868	1.3872	0.0937	1.9149
	<i>Initial Range : [-0.10,0.20]</i>													
	<i>Initial Range : [-0.15,0.10]</i>													
Nitrogen - Carbon dioxide	46	220.000	14.8927–136.1559	8	-0.0250	2.9816	-0.0076	3.7337	-0.0250	3.0207	-0.0736	2.8921	0.0497	4.7297
	46	240.000	20.7254–142.8275	14	-0.0319	2.6788	-0.0163	3.2371	-0.0337	2.7158	-0.1101	2.9115	0.0410	4.8613
	47	270.000	39.0000–95.0000	18	-0.0128	0.5846	-0.0007	0.8880	-0.0181	0.8321	-0.1500	0.8138	0.0670	1.4617

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Table 4.9 Binary interaction parameters and percent AAD for systems containing CO₂ of five equations of state using the fugacity criterion

SYSTEM	Ref	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Carbon dioxide – Methane	46	219.260	13.7952–38.1051	5	0.1083	2.3385	0.1083	2.5618	0.1042	2.3762	0.1028	2.6092	0.1208	2.7561
	48	230.000	15.0000–69.0800	13	0.1042	2.4918	0.1042	2.9942	0.1000	5.0184	0.0972	3.4211	0.1167	4.9269
	46	240.000	20.7649–74.9470	10	0.0972	1.3930	0.0958	1.8826	0.0917	1.3707	0.0847	2.1380	0.1056	3.4416
	48	250.000	20.0000–77.0000	8	0.1028	2.3961	0.1000	2.4646	0.0958	2.1496	0.0861	2.2816	0.1153	6.8929
	Initial Range : [0.00,0.20]	46	270.000	36.2497–69.9038	7	0.1208	0.9984	0.1153	0.6929	0.1111	0.3282	0.1000	0.6729	0.1292
Carbon dioxide – Ethane	48	250.000	14.2300–18.5100	13	0.1292	0.9351	0.1250	1.1774	0.1308	1.0997	0.1319	1.3370	0.1236	1.5256
	Initial Range : [0.00,0.20]													
Carbon dioxide – Propane	49	244.271	4.9674–13.4051	10	0.1347	1.8912	0.1264	1.5988	0.1292	1.7776	0.1250	2.0608	0.1250	2.0608
	49	266.493	7.9614–25.7894	11	0.1319	2.0942	0.1264	2.0135	0.1308	2.0318	0.1264	2.1442	0.1264	2.1442
Carbon dioxide – n-Butane	50	368.160	15.1098–70.0913	8	0.1869	2.7848	0.1722	2.5622	0.1764	2.3592	0.1792	1.8957	0.1736	2.2330
	50	393.160	23.6072–43.4148	5	0.2153	2.4012	0.1972	2.4735	0.1986	1.9874	0.1972	1.3077	0.1972	2.0911
Carbon dioxide – i-Butane	51	310.836	7.1448–55.1853	8	0.1308	1.0980	0.1222	1.3482	0.1264	1.1748	0.1292	1.2008	0.1236	1.4048
	51	344.271	21.3664–61.7858	6	0.1528	0.9308	0.1417	1.1717	0.1458	0.8365	0.1472	0.5170	0.1458	1.1084
Carbon dioxide – n-Pentane	52	277.660	2.2455–7.0170	10	0.1514	6.3384	0.1444	6.0446	0.1444	5.8692	0.1528	6.1272	0.1444	6.1226
	52	311.049	4.5591–61.5136	10	0.1319	3.8183	0.1250	3.9944	0.1250	3.9168	0.1319	3.8636	0.1250	3.9201
	52	344.160	4.0828–88.4548	14	0.1639	5.3585	0.1514	5.4858	0.1514	5.3681	0.1587	5.3673	0.1514	5.3475
	52	377.604	8.9821–87.5072	8	0.1653	3.4476	0.1486	3.5905	0.1486	3.5512	0.1556	3.6124	0.1500	3.6418
	53	408.160	13.8169–71.9270	7	0.2222	6.7621	0.1972	6.4847	0.1972	6.3052	0.2069	6.4152	0.1986	6.5568
Initial Range : [0.10,0.30]	53	436.160	21.7715–58.3173	5	0.2903	4.7447	0.2597	4.2373	0.2569	4.3600	0.2639	4.2009	0.2611	4.2955
Carbon dioxide – i-Pentane	53	408.160	15.9191–71.7197	9	0.2236	5.1059	0.1986	4.8516	0.2014	4.7978	0.2083	4.9727	0.2014	4.8375
	Initial Range : [0.10,0.30]													
Carbon dioxide – n-Heptane	54	310.660	8.7099–52.9398	10	0.1236	2.7136	0.1139	2.6498	0.1089	2.5755	0.1236	2.6645		
	54	352.604	4.1848–114.5895	14	0.1125	0.8007	0.1028	1.0890	0.0944	1.1666	0.1083	0.9190		
	54	394.271	11.1595–130.6483	15	0.1111	2.8071	0.1000	3.8389	0.0903	4.0963	0.0972	2.5186		
	54	477.216	17.2837–95.8088	6	0.1556	3.1357	0.1319	4.1659	0.1153	4.0362	0.1097	3.2224		
Carbon dioxide – n-Decane	55	462.560	19.3600–50.7000	4	0.1444	1.2087	0.1167	1.5624	0.0750	1.5089	0.1083	0.8242		
	55	476.960	14.2500–50.1000	4	0.1472	0.9349	0.1167	1.3290	0.0750	1.7048	0.1056	0.9245		
	55	542.960	29.3800–51.0000	4	0.2222	1.7306	0.1750	2.5549	0.1194	2.5223	0.1278	1.2845		
Initial Range : [0.00,0.40]	55	583.660	19.7800–50.4000	4	0.3722	2.0881	0.3139	3.2404	0.2528	3.1089	0.2404	1.5933		

Table 4.10 Binary interaction parameters and percent AAD for systems containing CO₂ of five equations of state using the bubble point pressure criterion

SYSTEM	Ref.	T (K)	Range of P (atm)	N	SRK EOS		PR EOS		PT EOS		MSRK EOS		MPR EOS	
					K _{ij}	AAD(%)								
Carbon dioxide – Methane	46	219.260	13.7952–38.1051	5	0.1069	2.4055	0.1069	2.6318	0.1028	2.4478	0.1014	2.6775	0.1167	2.9602
	46	230.000	15.0000–69.0800	13	0.0944	1.1068	0.0944	1.2295	0.0917	1.0651	0.0847	1.5365	0.1014	2.7264
	46	240.000	20.7649–74.9470	10	0.0966	1.4640	0.0358	1.8860	0.0944	1.5050	0.0847	2.1390	0.1028	3.3308
	46	250.000	20.0000–77.0000	8	0.0989	0.8097	0.0889	1.4009	0.0861	1.2063	0.0750	1.4160	0.0966	2.1846
	46	270.000	36.2497–69.9038	7	0.1139	0.3358	0.1097	0.2474	0.1063	0.2118	0.0944	0.2965	0.1250	0.4816
	<i>Initial Range : [0.00, 0.20]</i>													
Carbon dioxide – Ethane	48	250.000	14.2300–18.5100	13	0.1347	0.4264	0.1319	0.4237	0.1375	0.4218	0.1403	0.4893	0.1319	0.6448
	<i>Initial Range : [0.00, 0.20]</i>													
Carbon dioxide – Propane	49	244.271	4.9674–13.4051	10	0.1333	1.8972	0.1278	1.6438	0.1333	1.6395	0.1347	1.6864	0.1278	2.0644
	49	266.493	7.9614–25.7894	11	0.1361	2.0499	0.1292	1.9755	0.1347	1.9822	0.1375	2.0151	0.1306	2.0414
Carbon dioxide – n-Butane	50	368.160	15.1098–70.0913	8	0.1653	0.7126	0.1500	0.6260	0.1558	0.6809	0.1597	0.6827	0.1528	0.7056
	50	383.160	23.6072–43.4148	5	0.1736	0.6158	0.1558	0.3350	0.1639	0.3009	0.1722	0.2379	0.1597	0.2739
Carbon dioxide – i-Butane	51	310.938	7.1448–55.1853	8	0.1292	0.9863	0.1194	1.1046	0.1500	5.1186	0.1292	1.2008	0.1236	1.4046
	51	344.271	21.3664–61.7858	6	0.1486	0.6797	0.1347	0.5886	0.1417	0.5703	0.1458	0.4329	0.1403	0.5560
Carbon dioxide – n-Pentane	52	277.660	2.2455–7.0170	10	0.1375	5.5250	0.1306	5.1014	0.1319	5.0153	0.1389	5.2405	0.1306	5.1698
	52	311.049	4.5581–61.5136	10	0.1361	4.3997	0.1278	4.4485	0.1278	4.3637	0.1361	4.4643	0.1278	4.3730
	52	344.160	4.0628–88.4548	14	0.1403	2.4229	0.1292	2.6225	0.1306	2.7673	0.1375	2.6635	0.1292	2.5209
	52	377.604	8.9821–87.5072	8	0.1569	2.4381	0.1403	2.5496	0.1417	2.6668	0.1486	2.8506	0.1417	2.5606
	53	408.160	13.8169–71.9270	7	0.1784	3.4394	0.1558	3.3748	0.1569	3.4142	0.1625	3.5856	0.1569	3.3923
	53	436.160	21.7715–58.3173	5	0.2167	0.5352	0.1903	0.8187	0.1903	0.5425	0.1944	0.3502	0.1917	0.8453
Carbon dioxide – i-Pentane	53	408.160	15.9191–71.7197	9	0.1694	1.2178	0.1500	1.2907	0.1528	1.4259	0.1542	1.7084	0.1528	1.3493
	<i>Initial Range : [0.10, 0.30]</i>													
Carbon dioxide – n-Heptane	54	310.660	8.7099–52.9398	10	0.1181	2.4220	0.1097	2.4319	0.1028	2.3159	0.1194	2.4279		
	54	352.604	4.1848–114.5895	14	0.1125	0.8007	0.1014	0.8984	0.0917	0.8510	0.1083	0.9190		
	54	394.271	11.1595–130.8483	15	0.0972	2.1299	0.0833	2.3156	0.0722	2.4480	0.0847	1.8471		
	54	477.216	17.2837–95.8088	6	0.1236	0.7977	0.1042	2.2480	0.0903	2.3482	0.0750	0.4455		
Carbon dioxide – n-Decane	55	462.560	19.3600–50.7000	4	0.1369	0.7316	0.1083	0.8856	0.0887	0.9674	0.1028	0.8965		
	55	476.960	14.2500–50.1000	4	0.1417	0.7730	0.1083	0.9832	0.0839	1.1181	0.1000	0.7152		
	55	542.960	29.3800–51.0000	4	0.2028	0.8503	0.1500	0.9885	0.0944	1.0723	0.1111	0.7606		
	55	583.660	19.7600–50.4000	4	0.3361	1.2743	0.2611	1.4199	0.2028	1.5287	0.2139	1.1174		
<i>Initial Range : [0.00, 0.40]</i>														

4.2 Vapor-Liquid Equilibrium Calculations

The application of the rapid fugacity method was intended to indicate its advantage of less computation time. In addition, the optimum K_{ij} values predicted from the minimization of the deviation in bubble point pressure method certainly yielded better result in bubble point calculations. Therefore, in the VLE prediction part, the optimum K_{ij} values from the bubble point pressure method would be used to evaluate the bubble point pressure and vapor phase composition for each data set in all systems. These results are also given in details in Appendix B

Additionally, taken from these VLE results, the isotherm pressure-composition diagrams at two different temperatures from experimental data and those evaluated by five equations of state for each system are shown in Figure 4.1 for systems containing methane, Figure 4.2 for systems containing ethane, Figure 4.3 for systems containing propane, Figure 4.4 for systems containing nitrogen and Figure 4.5 for systems containing carbon dioxide.

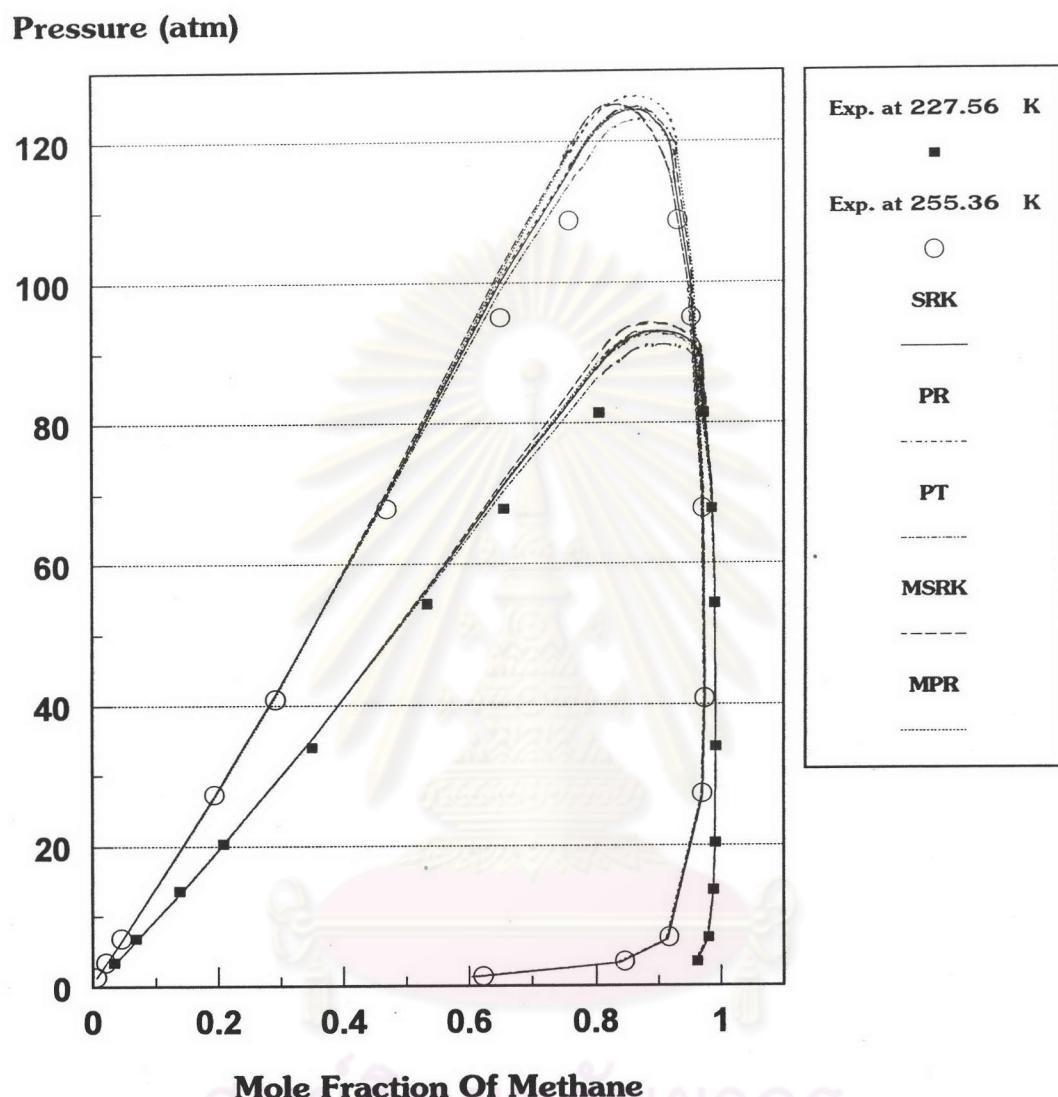


Figure 4.1 Comparison of calculated and experimental VLE for Methane - n-Butane system at 227.56 K and 255.36 K

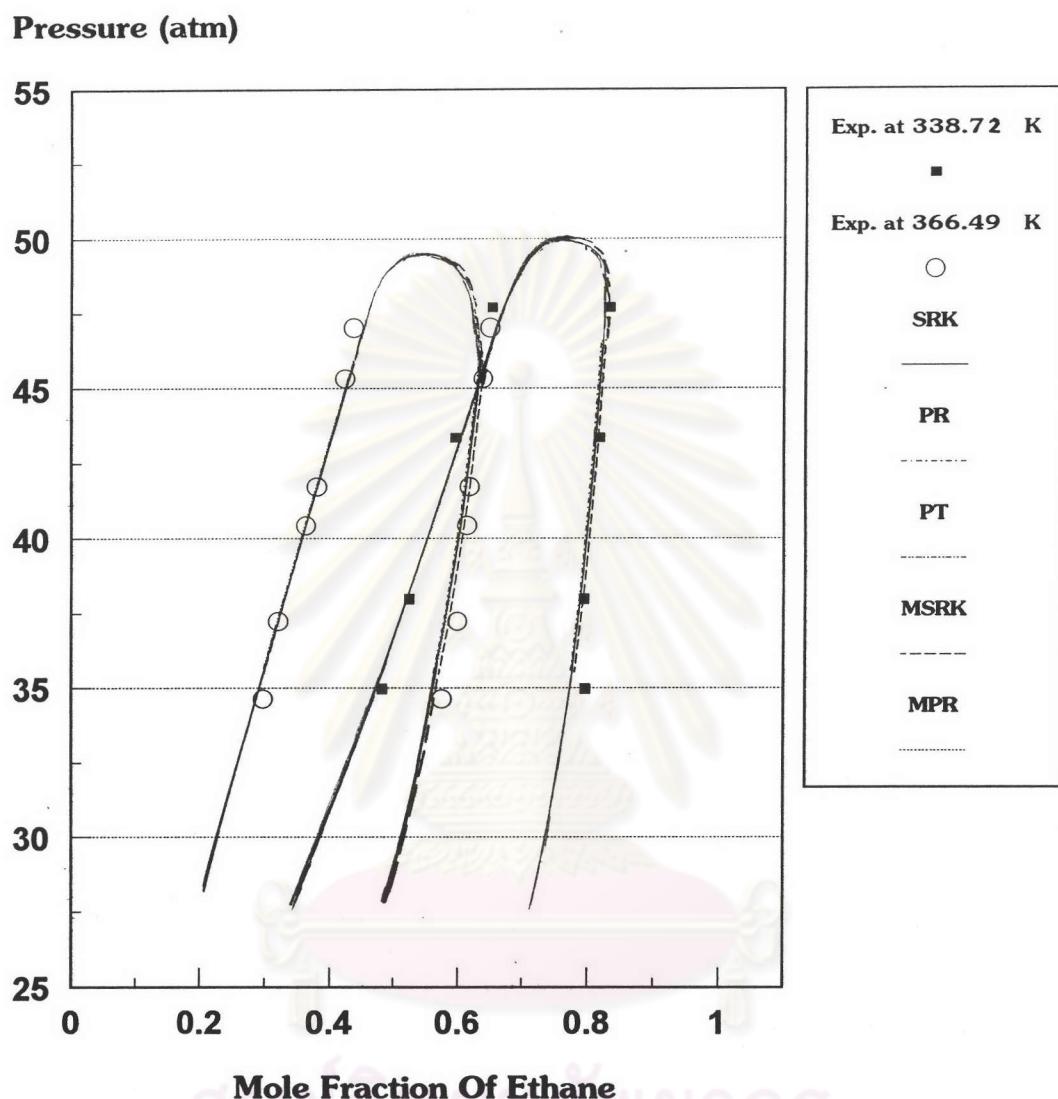


Figure 4.2 Comparison of calculated and experimental VLE for Ethane - n-Butane system at 338.72 K and 366.49 K

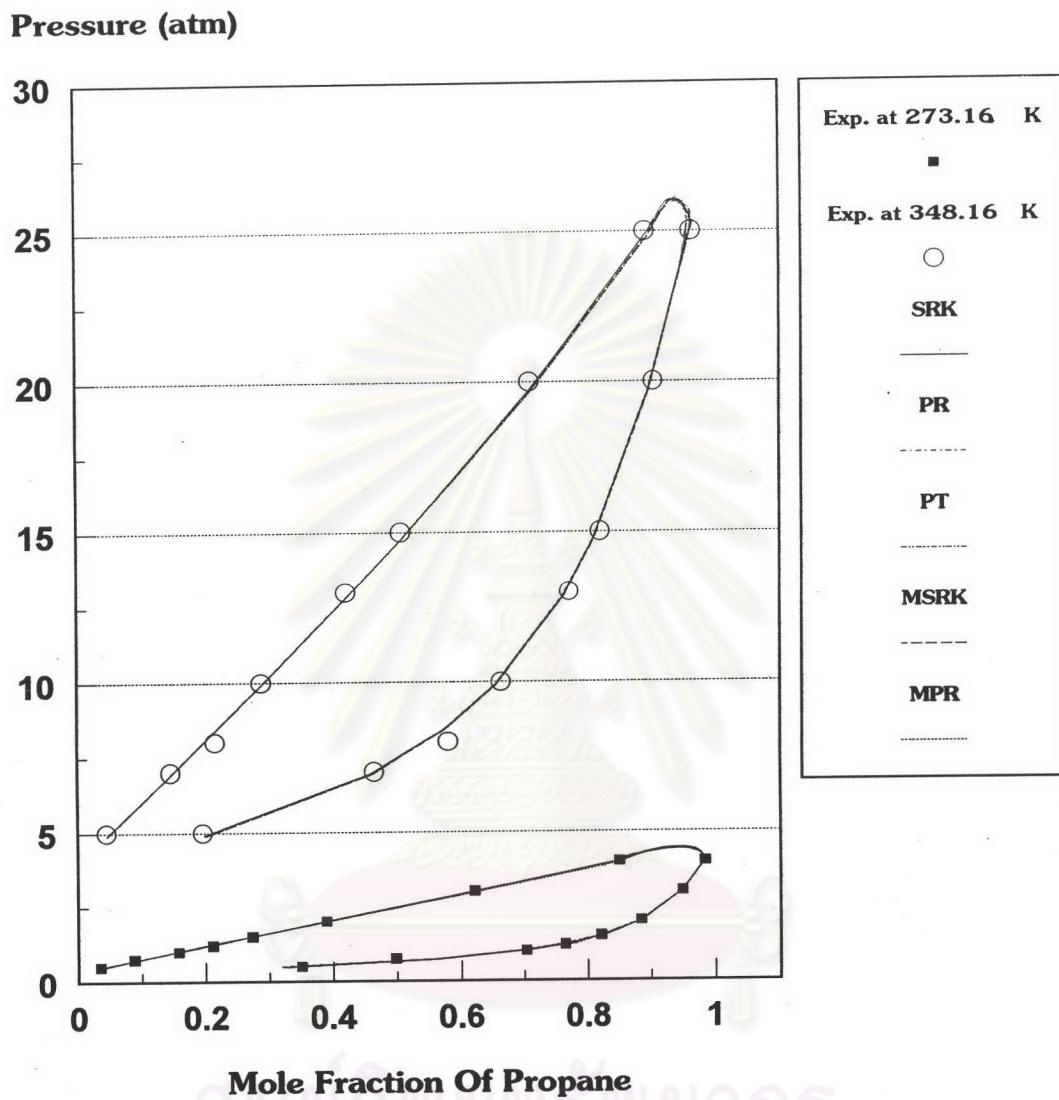


Figure 4.3 Comparison of calculated and experimental VLE for Propane - Isopentane system at 273.16 K and 348.16 K

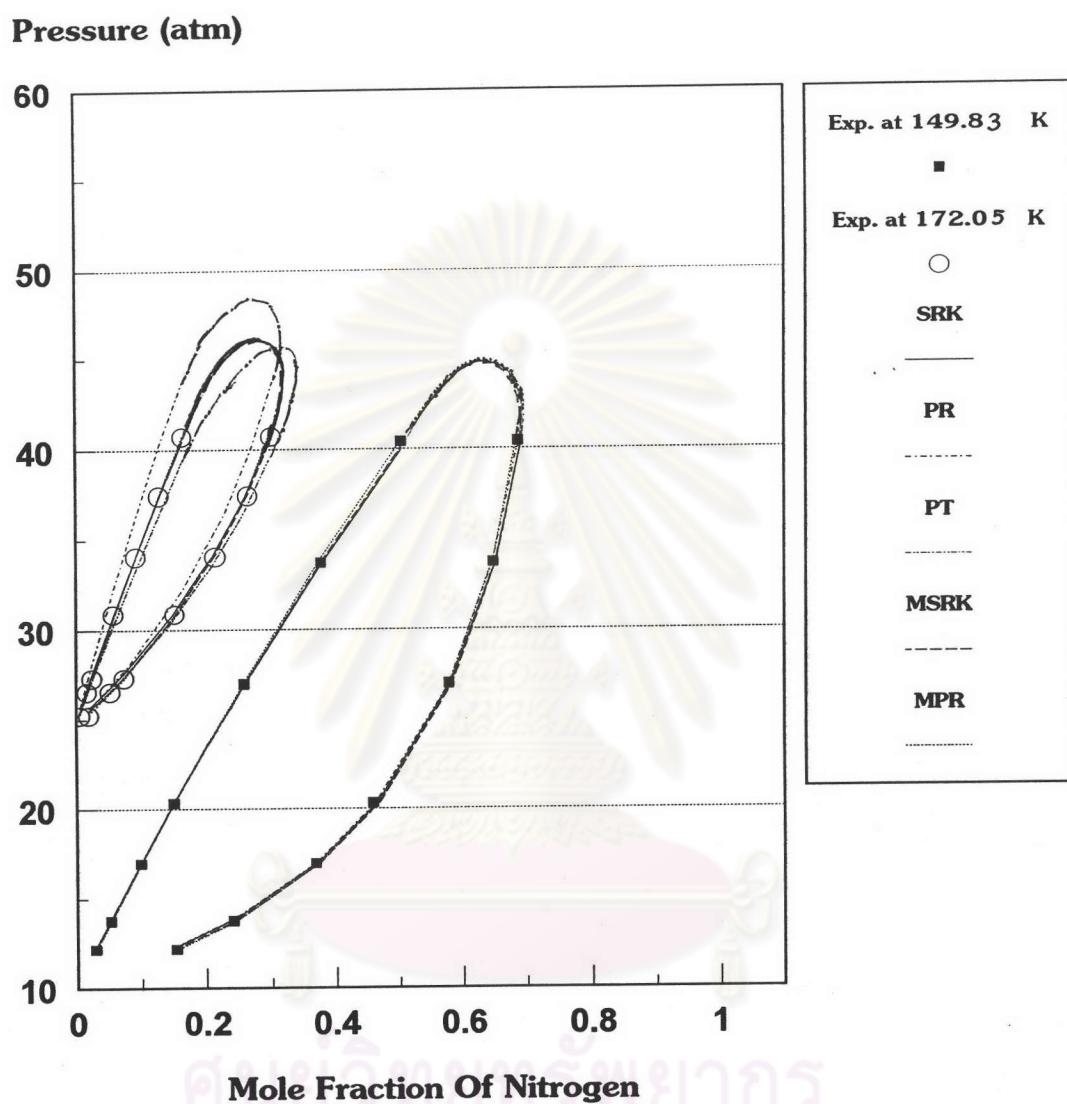


Figure 4.4 Comparison of calculated and experimental VLE for Nitrogen -Methane system at 149.83 K and 172.05 K

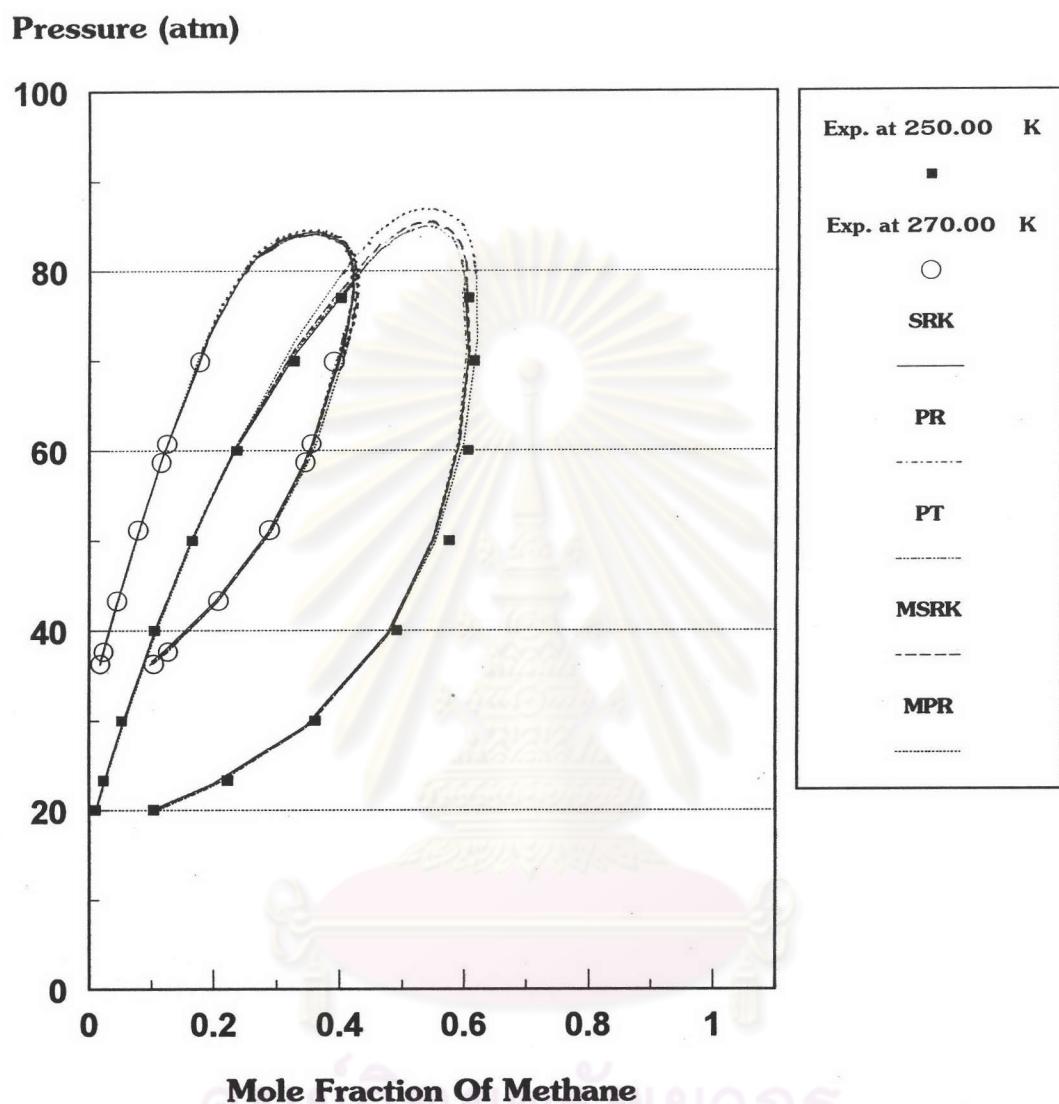


Figure 4.5 Comparison of calculated and experimental VLE for Carbon dioxide - Methane system at 250.00 K and 270.00 K