Supplementary Material of “Functional-Segment Activity Coefficient model: F-SAC”

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VLE type description:

[1] Mixtures with IDAC values considered in the fit.

[2] Mixtures not considered in the parameter fit.

[3] Mixtures of fuctinal groups with IDAC values not considered in the parameter fit.

[4] Mixtures with IDAC values not considered at all in the fit.

List of references for this document

{1} Paul,H.I., J.Krug, B.Gutsche and H.Knapp, J.Chem.Eng.Data, 31, 448 (1986)
{2} Paul,H.I., J.Krug and H.Knapp, J.Chem.Eng.Data, 33, 453 (1988)
{3} LAURANCE,D.R. and G.W.SWIFT, J.Chem.Eng.Data, 19, 61 (1974)
{4} Lozano,L.M., e.A.Montero, M.C.Martin and M.A.Villamanan, Fluid Phase Equilib., 133, 155 (1997)
{5} Jagjit R. Khurma, J.Chem.Eng.Data, 28, 86-93 (1983)
{6} Lee,M.J. and C.H.Hu, Fluid Phase Equilib., 109, 83 (1995)
{7} Maria Antosik, Maria GaLka, and StanisLaw K. Malanowski, J. Chem. Eng. Data, Vol. 49, No. 1, 2004
{8} Jean-Pierre Monfort, J.Chem.Eng.Data, 28, 24-27 (1983)
{9} Tetsuo Morisue, Katsuji Noda and Kiyoharu Ishida, J. Chem. Eng. Japan, 4, 355 (1973)
{10} Goral,M., Fluid Phase Equilib., 102, 275 (1994)
{11} Bissell,T.G. and A.G.Williamson, J.Chem.Thermodyn., 7, 131 (1975)
{12} Dahmani,O., I.Wichterle and A.Ait-Kaci, Fluid Phase Equilib., 124, 135 (1996)
{13} Jagjit R. Khurma, Ol Muthu, Sarat Munjal and Burford, J.Chem.Eng.Data, 28, 412 (1983)
{14} Treszczanowicz,T. and B.C.-Y.Lu, J.Chem.Thermodyn., 18, 213 (1986)
{15} Pozo de Fernandez,M.E., J.C.G.Calado, J.A.Zollweg and W.B.Streett, Fluid Phase Equilib., 74, 289 (1992)
{16} Campbell,S.W., R.A.Wilsak and G..Thodos, J.Chem.Eng.Data, 31, 424 (1986)
{17} Jurgen Gmehling, J.Chem.Eng.Data, 28, 27-30 (1983)
{18} Muthu,Ol., Patri.J..Maher and Bufor.D..Smith, J.Chem.Eng.Data, 25, 163 (1980)
{19} Wu,H.S. and S.I.Sandler, J.Chem.Eng.Data, 33, 157 (1988)
{20} Shealy,G.S., T.J.Bauer, T..Hauschild and S.I.Sandler, J.Chem.Eng.Data, 31, 457 (1986)
{21} Pena,M.D., A.C.Colin and A..Compostizo, J.Chem.Thermodyn., 10, 1101 (1978)
{22} Pena,M.D., A.C.Colin and A..Compostizo, J.Chem.Thermodyn., 10, 337 (1978)
{23} Mato,F.A. and C.Berro, J.Chem.Eng.Data, 36, 262 (1991)
{24} Shealy,G.S. and S.I.Sandler, J.Chem.Eng.Data, 30, 455 (1985)
{25} Scheller,W.S., A.R.Torres-soto and K.J.Daphtary, J.Chem.Eng.Data, 14, 17 (1969)
{26} Jagjit R. Khurma, Ol Muthu, Sarat Munjal and Burford, J.Chem.Eng.Data, 28, 412 (1983)
{27} Campbell,S.W., R.A.Wilsak and G..Thodos, J.Chem.Eng.Data, 31, 424 (1986)
{28} J. W. Glanville, B.H.Sage andW. N. Lacey, Ind.Eng.Chem.Data, 508,513 (1950)
{29} Ohgaki,K., H.Takata, T.Washida and T.Katayama, Fluid Phase Equilib., 43, 105 (1988)
{30} Stanley J Ashcroft, Andrew D Clayton and Ronald B Shearn, J.Chem.Eng.Data, 24, 195 (1979)
{31} Naumann,D. and H.G.Wagner, J.Chem.Thermodyn., 18, 81 (1986)
{32} Colin,A.C., A.Compostizo and M.Pena, J.Chem.Thermodyn., 16, 497 (1984)
{33} International Conference on Distillation & Absorption, Kongresshaus, Baden-Baden, Germany 09/2002
{34} PAUL,H.I., J.KRUG and H.KNAPP, Fluid Phase Equilib., 39, 307 (1988)
{35} Humphrey,J.L. and M.Van Winkle, J.Chem.Eng.Data, 12, 526 (1967)
{36} Teodorescu,M., A.Barhala, D.Marchidan and O.Landauer, Fluid Phase Equilib., 126, 127 (1996)
{37} Willman,B. and A.S.Teja, J.Chem.Eng.Data, 30, 116 (1985)
{38} Pozo de Fernandez,M.E., J.Noles, J.Zollweg and W.B.Streett, Fluid Phase Equilib., 36, 91 (1987)
{39} SASSA,Y., R.KONISHI and T.KATAYAMA, J.Chem.Eng.Data, 19, 44 (1974)
{40} Shealy,G.S. and S.I.Sandler, J.Chem.Thermodyn., 17, 143 (1985)

				F-SAC		UNIFAC		COSMO-SAC		
Type	Mixture	T (K)	NP	ΔP (%)	Δy (%)	ΔP (%)	Δy (%)	ΔP (%)	Δy (%)	Ref.
[1]	1,1,1-trichloroethane/di-n-butyl ether	323.15	21	1.12%	0.41%	1.66%	0.21%	0.87%	0.34%	{1}
[1]	1,1,1-trichloroethane/di-n-butyl ether	343.15	23	1.25%	0.32%	1.83%	0.22%	1.12%	0.28%	{1}
[1]	acetone/1-chlorobutane	298.16	11	1.59%	0.15%	3.28%	0.84%	1.64%	0.94%	{5}
[1]	acetone/1-chlorobutane	348.16	11	0.98%	0.76%	2.11%	0.49%	2.32%	1.22%	{5}
[1]	acetone/1-chlorobutane	398.17	11	2.07%	1.89%	1.68%	1.42%	2.62%	1.97%	{5}
[1]	acetone/cyclohexane	323.15	27	0.62%	0.86%	3.10%	0.53%	4.27%	2.02%	{32}
[1]	acetone/benzene	323.15	25	0.24%	0.57%	1.82%	0.57%	5.95%	2.22%	{21}
[1]	benzene/n-hexane	313.15	17	0.34%	0.30%	1.10%	0.45%	6.25%	2.66%	{10}
[1]	benzene/n-octane	313.15	15	0.42%	0.29%	0.39%	0.36%	6.94%	1.44%	{10}
[1]	carbon tetrachloride/n-heptane	298.15	14	0.38%	0.13%	0.42%	0.11%	3.72%	1.16%	{11}
[1]	chloroform/n-hexane	298.15	15	1.62%	0.31%	1.20%	0.12%	1.88%	0.72%	{11}
[1]	chloroform/n-hexane	318.15	11	1.78%	0.51%	1.06%	0.28%	1.37%	0.58%	{11}
[1]	chloroform/n-hexane	328.15	11	2.57%	0.61%	1.65%	0.37%	0.66%	0.45%	{11}
[1]	chloroform/n-heptane	298.20	13	2.29%	0.46%	1.65%	0.34%	0.94%	0.33%	{11}
[1]	methyl ethyl ketone/cyclohexane	323.15	32	1.36%	1.16%	0.57%	0.67%	0.78%	0.50%	{32}
[1]	diisopropyl ether/benzene	343.15	16	1.77%	0.34%	0.81%	0.17%	4.04%	1.16%	{14}
[1]	diisopropyl ether/n-heptane	323.15	14	1.65%	0.84%	0.74%	0.54%	1.16%	0.72%	{14}
[1]	diisopropyl ether/n-heptane	343.15	15	1.74%	1.18%	0.46%	0.99%	1.25%	1.12%	{14}
[1]	dimethyl sulfoxide/benzene	293.15	11	2.42%	0.96%	1.70%	0.95%	137.74%	1.41%	{33}
[1]	dimethyl sulfoxide/benzene	323.15	11	1.72%	0.24%	1.31%	0.24%	128.32%	0.97%	{33}
[1]	dimethyl sulfoxide/benzene	363.15	11	2.04%	0.08%	0.91%	0.10%	116.33%	2.30%	{33}
[1]	ethyl acetate/1-chlorobutane	298.15	11	1.58%	0.40%	1.71%	0.46%	2.22%	1.09%	{5}
[1]	ethyl acetate/cyclohexane	313.15	17	1.00%	0.33%	0.57%	0.42%	6.39%	2.81%	{19}
[1]	methyl ethyl ketone/benzene	323.15	35	1.56%	0.44%	0.15%	0.31%	2.47%	1.07%	{21}
[1]	n-heptane/chlorobenzene	323.15	18	0.55%	0.48%	1.34%	0.85%	8.77%	3.22%	{34}
[1]	n-heptane/chlorobenzene	343.15	12	0.82%	0.45%	1.02%	0.56%	6.17%	1.93%	{34}
[1]	toluene/methyl ethyl ketone	323.15	28	0.88%	0.49%	1.68%	0.75%	3.36%	1.26%	{22}
[1]	methyl ethyl ketone/toluene	330.15	15	0.58%	0.39%	1.79%	0.49%	3.18%	0.80%	{31}
[1]	p-xylene/n-hexane	313.15	16	0.95%	0.16%	4.15%	0.52%	4.37%	0.86%	{10}
[1]	p-xylene/n-heptane	313.15	14	0.34%	0.14%	2.62%	0.67%	3.30%	1.07%	{10}
[1]	p-xylene/n-decane	313.15	24	1.78%	0.33%	1.99%	0.38%	1.92%	1.16%	{10}
[1]	tetrahydrofuran/cyclohexane	313.15	24	1.27%	0.49%	0.71%	0.26%	0.48%	0.19%	{19}
[1]	tetrahydrofuran/cyclohexane	333.15	21	0.97%	0.57%	0.78%	0.23%	0.34%	0.25%	{19}
[1]	tetrahydrofuran/ethyl acetate	313.15	16	2.09%	0.97%	3.01%	1.40%	0.76%	0.48%	{19}
[1]	tetrahydrofuran/ethyl acetate	333.15	16	2.37%	1.01%	3.37%	1.41%	0.91%	0.45%	{19}
[1]	toluene/n-hexane	313.15	10	0.59%	0.33%	2.84%	0.79%	5.17%	1.47%	{19}
[1]	toluene/n-heptane	313.15	17	0.68%	0.29%	1.06%	0.57%	4.67%	1.81%	{30}
[1]	toluene/n-decane	313.15	13	0.75%	0.28%	1.56%	0.18%	4.78%	1.09%	{10}
[1]	toluene/n-decane	373.50	12	4.17%	0.78%	3.39%	0.69%	1.55%	0.49%	{10}
[1]	toluene/n-decane	383.60	11	1.94%	0.53%	1.95%	0.57%	2.97%	0.69%	{10}
[1]	triethylamine/n-hexane	333.15	9	0.51%	0.64%	0.61%	0.61%	0.88%	0.74%	{35}
[2]	1-chlorobutane/n-heptane	323.15	13	2.44%	1.09%	2.02%	0.94%	1.67%	0.80%	{12}
[2]	1-chlorobutane/toluene	298.16	11	0.57%	0.40%	1.46%	0.41%	0.88%	0.33%	{5}
[2]	1-chlorobutane/toluene	323.15	13	0.81%	0.39%	0.45%	0.26%	0.41%	0.27%	{12}
[2]	1-chlorobutane/toluene	348.18	11	0.40%	0.42%	0.39%	0.45%	0.37%	0.36%	{5}
[2]	1-chlorobutane/toluene	398.22	11	0.49%	0.72%	0.81%	0.85%	0.75%	0.67%	{5}
[2]	1-hexene/n-hexane	313.15	24	0.56%	0.23%	1.30%	0.26%	0.43%	0.26%	{4}
[2]	1,3-butadiene/n-butane	310.93	11	2.04%	0.44%	1.44%	0.75%	2.43%	0.59%	{3}
[2]	acetone/diisopropyl ether	343.26	11	1.28%	0.49%	3.38%	1.57%	2.77%	1.38%	{6}
[2]	acetone/diisopropyl ether	353.27	11	1.45%	0.59%	3.18%	1.63%	2.42%	1.35%	{6}
[2]	acetone/diisopropyl ether	363.29	11	2.40%	0.86%	2.02%	1.31%	1.21%	0.97%	{6}
[2]	benzene/n-decane	313.15	21	0.97%	0.07%	1.11%	0.05%	6.73%	0.53%	{10}
[2]	carbon tetrachloride/n-hexane	298.15	12	0.93%	0.49%	1.08%	0.48%	3.37%	1.19%	{11}
[2]	dimethyl ether/n-butane	282.96	21	1.36%	2.22%	0.56%	2.33%	3.07%	2.87%	{15}
[2]	ethyl acetate/1-octene	348.15	25	4.51%	2.46%	1.69%	1.42%	16.56%	6.30%	{17}
[2]	ethyl acetate/cyclohexane	313.15	17	1.00%	0.33%	0.57%	0.42%	6.39%	2.81%	{19}
[2]	ethylbenzene/cyclooctane	343.15	15	1.14%	0.25%	0.59%	0.40%	1.76%	0.75%	{36}
[2]	ethylbenzene/cyclooctane	353.15	14	0.78%	0.30%	0.52%	0.51%	1.64%	0.75%	{36}
[2]	ethylbenzene/cyclooctane	373.15	11	0.31%	0.18%	1.01%	0.41%	1.68%	0.59%	{36}
[2]	ethylbenzene/n-hexane	313.15	11	1.26%	0.25%	1.43%	0.34%	6.74%	1.66%	{10}
[2]	ethylbenzene/n-heptane	313.15	15	1.26%	0.36%	1.49%	0.55%	5.70%	2.04%	{10}
[2]	ethylbenzene/n-octane	313.15	13	0.90%	0.16%	1.22%	0.25%	4.36%	1.61%	{10}

[2]	ethylbenzene/n-decane	313.15	19	0.82%	0.79%	1.74%	1.03%	5.24%	2.06%	{10}
[2]	methyl n-propyl ketone/benzene	323.15	25	1.74%	4.22%	0.32%	4.28%	1.68%	4.71%	{21}
[2]	n-butyl acetate/1-decene	363.15	35	3.02%	1.43%	0.81%	0.72%	9.25%	3.11%	{17}
[2]	n-heptane/n-butyl acetate	373.15	18	1.23%	0.59%	2.60%	0.68%	3.71%	1.55%	{25}
[2]	n-heptane/n-butyl acetate	347.85	18	2.90%	1.34%	4.05%	1.05%	2.95%	2.57%	{25}
[2]	toluene/methyl n-propyl ketone	323.15	27	1.10%	0.33%	1.29%	0.59%	2.01%	0.82%	{22}
[2]	toluene/m-xylene	373.60	17	0.69%	0.62%	0.84%	0.65%	0.75%	0.63%	{37}
[2]	toluene/m-xylene	383.60	11	0.65%	0.63%	0.70%	0.63%	0.66%	0.63%	{37}
[3]	toluene/m-xylene	393.70	11	2.00%	0.75%	2.17%	0.77%	2.05%	0.76%	{37}
[3]	1-chloropentane/di-n-butyl ether	323.15	17	2.00%	0.61%	2.08%	0.68%	2.10%	0.69%	{1}
[3]	benzene/cyclohexene	273.15	14	3.40%	1.60%	1.52%	0.79%	2.93%	1.17%	{9}
[3]	benzene/cyclohexene	293.15	13	2.48%	1.46%	1.21%	0.58%	2.78%	0.88%	{9}
[3]	dimethyl ether/1-butene	283.60	6	0.51%	0.72%	0.62%	0.78%	5.30%	2.07%	{38}
[3]	dimethyl sulfoxide/ethyl acetate	298.15	11	3.38%	0.04%	1.86%	0.03%	36.39%	0.26%	{39}
[4]	methyl acetate/1-hexene	323.15	24	0.72%	0.58%	0.77%	0.30%	15.51%	7.35%	{17}
[4]	1-chlorohexane/ethylbenzene	323.15	18	2.26%	0.34%	0.57%	0.37%	1.78%	0.22%	{2}
[4]	1-chlorohexane/ethylbenzene	343.15	20	1.23%	0.30%	0.98%	0.32%	0.76%	0.19%	{2}
[4]	di-n-pentyl ether/n-undecane	404.15	10	2.48%	0.23%	2.04%	0.30%	2.45%	0.23%	{14}
[4]	isobutyraldehyde/ethyl acetate	313.15	18	0.94%	0.46%	0.65%	0.36%	1.20%	0.50%	{20}
[4]	isobutyraldehyde/ethyl acetate	333.15	18	0.55%	0.57%	0.64%	0.41%	0.88%	0.63%	{20}
[4]	isobutyraldehyde/n-heptane	335.00	17	2.34%	0.69%	2.43%	0.67%	2.86%	0.83%	{40}
[4]	methyl n-butyl ether/benzene	343.15	12	0.40%	0.28%	0.36%	0.13%	1.72%	0.38%	{14}
[4]	methyl n-butyl ether/n-heptane	343.15	12	1.43%	0.69%	0.81%	0.58%	1.79%	0.67%	{14}
[4]	methyl n-butyl ether/n-heptane	323.15	13	1.58%	0.74%	0.90%	0.61%	1.92%	0.64%	{14}