CORRECTIONS

Joanne L. Budzien, John D. McCoy, John G. Curro, Randall A. LaViolette, and Eric S. Peterson: The Solubility of Gases in Polyethylene: Integral Equation Study of Standard Molecular Models. Volume 31, Number 19, September 22, 1998, p 6669.

In the attractive component of the WCA decomposition of the potential defined by eq 2.9b, the cutoff was inadvertently programmed to be at σ_{AB} rather than the stipulated $2^{1/6}\sigma_{AB}$. Correcting the WCA calculation changes a number of tables and figures: the corrected ones (Tables 1, 6, and 7 and Figures 2 and 3) are presented here.

Table 1. Potential Parameters and Solubility Coefficient Ratio S_{PRISM}/S_{MD} (%) for Comparison with the Molecular Dynamics Study Reported by van der Vegt et al.[11]

gases	σ (Å)	ϵ (K)	S_{PRISM}/S_{MD}(BH)	S_{PRISM}/S_{MD}(WCA)	S_{PRISM}/S_{MD}(av of BH and WCA)
N_2	3.70	95	59 ± 7	130 ± 10	95
Ar	3.40	120	50 ± 5	88 ± 9	69
O_2	3.50	110	57 ± 6	120 ± 10	88
CH_4	3.73	150	63 ± 8	152 ± 9	107
CH_2	3.93	47			

Table 6. Comparison of Solubility with Experimental Data[5] as S_{PRISM}/S_{exp} (%)[a]

a. NERD CH_2 Potential[8]

gas	N_2	Ar	O_2	CH_4	Kr	Xe	CO_2	C_2H_6
T_c(K)	126	150.8	154.8	191	209.4	289.4	304	305.42
HCB WCA	175	169	148	122	158	113	106	157
av	142	142	127	97	127	83	75	123
2HCB BH	109	115	105	72	95	53	43	89
BAH WCA	178	159		103	126	136	319	206
av	148	136		81	100	106	244	143
BAH BH	118	112		59	74	75	169	79
VHCB WCA	158	185	155	91	237	130	106	153
av	130	155	129	70	186	97	85	109
VHCB BH	101	124	103	49	134	64	63	65
MS WCA	220	161	172	199	180	221	331	
av	183	142	142	161	142	162	256	
MS BH	146	122	112	123	103	102	180	

b. TRaPPE CH_2 Potential[9]

gas	N_2	Ar	O_2	CH_4	Kr	Xe	CO_2	C_2H_6
T_c(K)	126	150.8	154.8	191	209.4	289.4	304	305.4
2HCB WCA	172	173	142	125	159	133	109	169
av	121	127	106	85	112	81	66	113
2HCB BH	69	80	70	45	64	29	22	56
BAH WCA	176	162		99	127	146	362	255
av	127	121		68	88	97	237	150
BAH BH	77	79		37	49	47	111	45
VHCB WCA	155	185	155	90	240	140	112	165
av	111	137	114	60	165	89	75	99
VHCB BH	66	88	72	29	89	38	38	33
MS WCA	218	159	172	206	181	239	342	
av	158	124	126	143	125	150	231	
MS BH	98	89	80	79	68	60	119	

[a] The first letters indicate the gas parameters with 2HCB = second virial coefficient of Hirschfelder, Curtiss, and Bird,[4] BAH = Ben-Amotz and Herschbach,[17] VHCB = viscosity of Hirschfelder, Curtiss, and Bird,[4] and MS = Matyushov and Schmid.[18] The final letters indicate the method of potential decomposition with BH = Barker−Henderson, and WCA = Weeks−Chandler−Anderson. Average refers to the arithmetic mean of the WCA and BH values for that gas.

Table 7. Best Fit for Each Gas (Notation Same as Table 6) with Experimental[5] Values of S in Units of (cm^3(STP)/cm^3/cm Hg).

a. NERD CH_2 Potential[8]

gas	T_c (K)	S_{PRISM}/S_{exp} (%)	WCA gas sets	S_{PRISM}/S_{exp} (%)	BH gas sets	experi-mental
N_2	126	158	VHCB	101	VHCB	9.05E-04
Ar	150.8	159	BAH	112	BAH	2.13E-03
O_2	154.8	148	2HCB	103	VHCB	1.96E-03
CH_4	191	103	BAH	123	MS	4.67E-03
Kr	209.4	126	BAH	103	MS	6.41E-03
Xe	289.4	113	2HCB	102	MS	2.75E-02
CO_2	304	106	2HCB, VHCB	65	VHCB	1.30E-02
C_2H_6	305.4	153	VHCB	89	2HCB	2.72E-02

b. TRaPPE CH_2 Potential[9]

gas	T_c (K)	S_{PRISM}/S_{exp} (%)	WCA gas sets	S_{PRISM}/S_{exp} (%)	BH gas sets	experi-mental
N_2	126	155	VHCB	98	MS	9.05E-04
Ar	150.8	159	MS	89	MS	2.13E-03
O_2	154.8	142	2HCB	80	MS	1.96E-03
CH_4	191	99	BAH	79	MS	4.67E-03
Kr	209.4	127	BAH	89	VHCB	6.41E-03
Xe	289.4	133	2HCB	60	MS	2.75E-02
CO_2	304	109	2HCB	111	BAH	1.30E-02
C_2H_6	305.4	165	VHCB	56	2HCB	2.72E-02

c. Best Set for Each Potential when Averaging WCA and BH

gas	T_c (K)	S_{PRISM}/S_{exp} (%) NERD	av gas sets NERD	S_{PRISM}/S_{exp} (%) TRaPPe	av gas sets TRaPPe
N_2	126	130	VHCB	111	VHCB
Ar	150.8	136	BAH	121	BAH
O_2	154.8	127	2HCB	106	2HCB
CH_4	191	97	2HCB	85	2HCB
Kr	209.4	100	BAH	88,112	BAH, 2HCB
Xe	289.4	97	VHCB	97	BAH
CO_2	304	85	VHCB	75	VHCB
C_2H_6	305.4	109	VHCB	99	VHCB

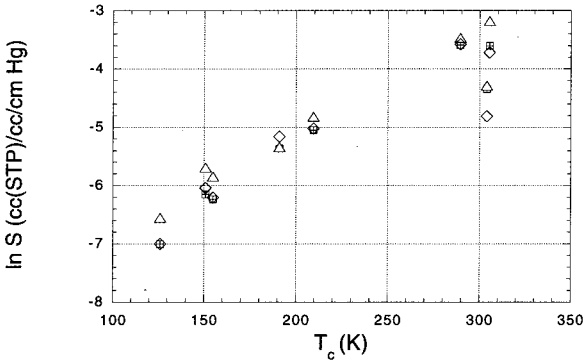

Figure 2. Solubility predictions for the best fit gases for the NERD potential.[8] The crossed squares are for amorphous polyethylene,[5] the triangles for the WCA separation, and the diamonds for the BH separation. See Table 7a for the best fit values and gas set.

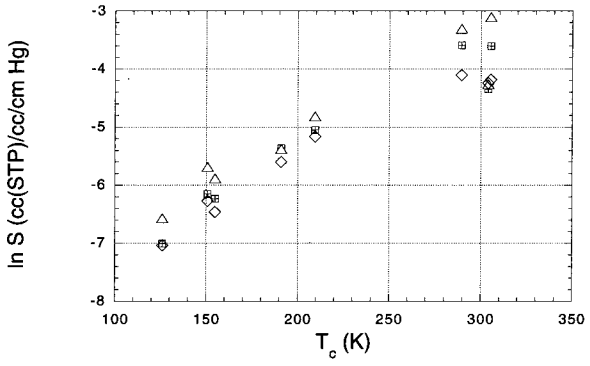

Figure 3. Solubility predictions for the best fit gases for the TRaPPE[9] potential. The crossed squares are for amorphous polyethylene,[5] the triangles for the WCA separation, and the diamonds for the BH separation. See Table 7b for the best fit values and gas set.

The conclusions of the study are also slightly changed. From the comparison with simulation, it appears that an average of the results of the WCA and BH separations works best. From the comparison to the alkane extrapolation, it is less clear what separation or combination works best in most cases. By judiciously selection of the gas from among the gas sets for a CH_2 parameter set with a given separation, the agreement is within 50% and is often much better. The results of the WCA decomposition are still fairly insensitive to the differences between the two CH_2 potentials while the BH decomposition can lead to large differences in the predicted solubilities.

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