Combination Look-up Table/Parameterization

general equation

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG
1	[Np]=10-6M, CO2=10-5 atm			lny=a+bx+cx^2+dx^3+ex^4+fx^5																													
2			Parameter	Values	Std Error	T Value	95% Conf	95% Conf Lim		XY #	X Observe	Y Observe	Y Predicte	Y Residual	Y Residual	95% Conf	95% Conf	95% Pred	95% Pred	First Deriv	Second De	Cum Area	FitRef		X Generate	Y Predicte	95% Conf	95% Conf	95% Pred	95% Pred	First Deriv	Second De	Cum Area
3	Eqn	lny=a+bx+c	a	923.2319	134.4258	6.867965	634.9171	1211.547		1*	2	0.234065	1.47E+80	-1.47E+80	-6.29E+82	1.47E+80	1.47E+80	1.47E+80	1.47E+80	-2.6E+82	4.62E+84	0			6	0.702931	0.532438	0.873424	0.478976	0.926885	0.482017	1.82299	0
4	Eqn #	6103	b	-632.0906	84.2415	-7.503316	-812.7706	-451.4105		2*	2.25	0.207848	5.03E+62	-5.03E+62	-2.42E+65	5.03E+62	5.03E+62	5.03E+62	5.03E+62	-7.33E+64	1.07E+67	8.36E+77			6.04798	0.728157	0.579888	0.876425	0.520621	0.935693	0.569563	1.82967	0.034315
5	r2	0.999933	c	172.1421	21.01241	8.192398	127.0749	217.2092		3*	2.5	0.207848	2.33E+48	-2.33E+48	-1.12E+51	2.33E+48	2.33E+48	2.33E+48	2.33E+48	-2.77E+50	3.32E+52	8.36E+77			6.09596	0.757598	0.628502	0.886695	0.563296	0.951901	0.657888	1.854907	0.069941
6	DF Adj r2	0.999902	d	-23.38039	2.608217	-8.964126	-28.97446	-17.78632		4*	2.75	0.207848	5.34E+36	-5.34E+36	-2.57E+39	5.34E+36	5.34E+36	5.34E+36	5.34E+36	-5.13E+38	4.97E+40	8.36E+77			6.143939	0.791313	0.678549	0.904077	0.607456	0.97517	0.747811	1.895923	0.107082
7	Fit Std Err	0.067706	e	1.587288	0.161148	9.849864	1.241659	1.932916		5*	3	0.207848	2.45E+27	-2.45E+27	-1.18E+30	2.45E+27	2.45E+27	2.45E+27	2.45E+27	-1.88E+29	1.45E+31	8.36E+77			6.191919	0.829395	0.730342	0.928448	0.653613	1.005177	0.840037	1.950532	0.145945
8	F-stat	41705.62	f	-0.043096	0.003966	-10.86769	-0.051601	-0.034591		6*	3.25	0.207848	9.93E+19	-9.93E+19	-4.78E+22	9.93E+19	9.93E+19	9.93E+19	9.93E+19	-5.97E+21	3.65E+23	8.36E+77			6.239899	0.871969	0.784238	0.959701	0.70231	1.041629	0.935174	2.01705	0.186742
9	Date	Apr 9, 1998								7*	3.5	0.207848	1.72E+14	-1.72E+14	-8.27E+16	1.72E+14	1.72E+14	1.72E+14	1.72E+14	-7.99E+15	3.79E+17	8.36E+77			6.287879	0.919189	0.840648	0.99773	0.754094	1.084284	1.033761	2.094178	0.229693
10	Time	3:14:05 PM								8*	3.75	0.234065	6.68E+09	-6.68E+09	-2.86E+12	6.68E+09	6.68E+09	6.68E+09	6.68E+09	-2.35E+11	8.54E+12	8.36E+77			6.335859	0.971232	0.900033	1.042431	0.8095	1.132963	1.136284	2.180935	0.275024
11										9*	4	0.234065	3310588	-3310588	-1.41E+09	3310579	3310596	3310579	3310596	-86175486	2.35E+09	8.36E+77			6.383838	1.028297	0.962898	1.093695	0.869034	1.187559	1.243186	2.276619	0.322972
12										10*	4.25	0.234065	12773.03	-12772.8	-5456938	12767	12779.07	12767	12779.07	-239020.2	4804379	8.36E+77			6.431818	1.090604	1.029779	1.151429	0.933164	1.248044	1.354883	2.38078	0.373783
13										11*	4.5	0.260335	251.0034	-250.743	-96315.41	246.8202	255.1866	246.8176	255.1891	-3254.244	47256.8	8.36E+77			6.479798	1.158394	1.101218	1.215569	1.002327	1.31446	1.471776	2.493177	0.427714
14										12*	4.75	0.286658	17.49702	-17.21036	-6003.788	14.68969	20.30435	14.68594	20.30811	-149.5078	1545.69	8.36E+77			6.527778	1.231924	1.177745	1.286104	1.076931	1.386918	1.594258	2.6138	0.485034
15										13*	5	0.313035	3.192989	-2.879954	-920.0108	1.38174	5.004237	1.375928	5.010049	-16.70192	123.5043	8.36E+77			6.575758	1.311474	1.259861	1.363087	1.157358	1.465589	1.722729	2.742831	0.546025
16										14*	5.25	0.365948	1.186812	-0.820864	-224.3117	0.073825	2.299799	0.064392	2.309232	-3.34894	19.03283	8.36E+77			6.623737	1.397339	1.348037	1.446641	1.243982	1.550696	1.857599	2.880634	0.610983
17										15*	5.5	0.445722	0.733299	-0.287577	-64.5194	0.090091	1.376506	0.073902	1.392695	-0.833469	4.991014	8.36E+77			6.671717	1.489838	1.442716	1.536959	1.337168	1.642508	1.999303	3.0278	0.680219
18										16*	5.75	0.552847	0.641539	-0.088693	-16.04288	0.297115	0.985964	0.267754	1.015325	-0.009194	2.282463	8.36E+77			6.719697	1.589308	1.544319	1.634297	1.437283	1.741333	2.148307	3.18507	0.754059
19										17	6	0.687991	0.702931	-0.01494	-2.171547	0.532438	0.873424	0.478976	0.926885	0.482017	1.82299	8.36E+77			6.767677	1.696113	1.653258	1.738968	1.544706	1.84752	2.305117	3.353375	0.832846
20										18	6.25	0.907131	0.881519	0.025612	2.823449	0.79589	0.967147	0.712937	1.050101	0.955625	2.032441	8.36E+77			6.815657	1.81064	1.769944	1.851335	1.659829	1.96145	2.470288	3.533795	0.916941
21										19	6.5	1.214444	1.188639	0.025805	2.124857	1.13279	1.244487	1.033054	1.344224	1.522643	2.542951	8.36E+77			6.863636	1.933304	1.894797	1.971811	1.78307	2.083539	2.644434	3.727645	1.006724
22										20	6.75	1.645098	1.655887	-0.010789	-0.655826	1.612244	1.69953	1.504254	1.807519	2.246403	3.289998	8.36E+77			6.911616	2.064553	2.028255	2.100851	1.914869	2.214237	2.828229	3.936259	1.102597
23										21	7	2.302181	2.330435	-0.028254	-1.227283	2.298201	2.36267	2.181685	2.479186	3.19461	4.364446	8.36E+77			6.959596	2.204866	2.170782	2.238951	2.055704	2.354029	3.022419	4.161209	1.204983
24										22	7.25	3.250673	3.280493	-0.029819	-0.917328	3.258523	3.302463	3.133624	3.427361	4.472329	5.963507	8.36E+77			7.007576	2.354762	2.322872	2.386652	2.206086	2.503439	3.227824	4.404063	1.314329
25										23	7.5	4.583925	4.60702	-0.023095	-0.503819	4.591627	4.622413	4.46099	4.75305	6.235966	8.267755	8.36E+77			7.055556	2.514801	2.485061	2.54454	2.366571	2.663031	3.445343	4.666459	1.431107
26										24	7.75	6.48362	6.453325	0.030295	0.467252	6.441466	6.465184	6.307626	6.599024	8.653411	11.10256	8.36E+77			7.103535	2.685585	2.657928	2.713243	2.537759	2.833412	3.675955	4.950093	1.55582
27										25	8	9.055447	8.989999	0.065448	0.722749	8.980968	8.99903	8.844503	9.135496	11.72687	13.12411	8.36E+77			7.151515	2.86777	2.842101	2.893439	2.720303	3.015237	3.920717	5.256567	1.688997
28										26	8.25	12.35283	12.32288	0.029958	0.242521	12.31627	12.32948	12.17751	12.46824	14.8245	10.30961	8.36E+77			7.199495	3.06206	3.038264	3.085857	2.914907	3.209213	4.180762	5.587402	1.831203
29										27	8.5	16.13444	16.23471	-0.100271	-0.62147	16.22926	16.24016	16.08939	16.38003	15.83421	-5.095739	8.36E+77			7.247475	3.269218	3.24716	3.291276	3.122336	3.4161	4.457294	5.94397	1.983037
30										28	8.75	19.68218	19.72458	-0.0424	-0.215423	19.71972	19.72944	19.57928	19.86987	10.6492	-39.34367	8.36E+77			7.295455	3.490064	3.469598	3.51053	3.343413	3.636715	4.751575	6.327378	2.145135
31										29	9	20.83294	20.72552	0.107424	0.515644	20.72084	20.7302	20.58023	20.87081	-4.248972	-76.94028	8.36E+77			7.343434	3.725482	3.706453	3.744511	3.579024	3.871939	5.064907	6.73823	2.318175
32										30	9.25	17.18213	17.17521	0.006921	0.04028	17.16897	17.18145	17.02986	17.32056	-23.72415	-65.99883	8.36E+77			7.391414	3.976417	3.958668	3.994166	3.83012	4.122713	5.398619	7.176831	2.502879
33										31	9.5	9.77604	9.904405	-0.128365	-1.313057	9.894011	9.914799	9.758817	10.04999	-31.01158	14.34052	8.36E+77			7.439394	4.243878	4.227258	4.260499	4.097714	4.390042	5.75403	7.642651	2.700015
34										32	9.75	3.481283	3.375895	0.105388	3.027283	3.345476	3.406313	3.227527	3.524262	-18.96136	67.1688	8.36E+77			7.487374	4.528939	4.513306	4.544571	4.382884	4.674993	6.132419	8.134366	2.910401
35										33	10	0.606738	0.55331	0.053429	8.805929	0.468745	0.637874	0.385265	0.721354	-4.991197	36.32793	8.36E+77			7.535354	4.832729	4.817962	4.847497	4.686764	4.978694	6.534976	8.649595	3.134909
36										34	10.25	0.05165	0.033809	0.01784	34.54093	-0.160522	0.228141	-0.208786	0.276405	-0.457969	5.505892	8.36E+77			7.583333	5.156436	5.14243	5.170442	5.010546	5.302325	6.962746	9.184586	3.374466
37										35	10.5	0	0.000566	-0.000566	0	-0.388647	0.38978	-0.414855	0.415988	-0.010992	0.198418	8.36E+77			7.631313	5.501288	5.487962	5.514614	5.355462	5.647114	7.416557	9.734037	3.630057
38										36	10.75	0	1.8E-06	-1.8E-06	0	-0.707402	0.707405	-0.722153	0.722157	-4.84E-05	0.001241	8.36E+77			7.679293	5.86855	5.855845	5.881256	5.72278	6.014321	7.896936	10.29058	3.902726
39										37*	11	0	7.1E-10	-7.1E-10	0	-1.196631	1.196631	-1.20541	1.20541	-2.57E-08	9E-07	8.36E+77			7.727273	6.259502	6.247377	6.271627	6.113781	6.405223	8.404002	10.8446	4.19358
40										38*	11.25	0	2.1E-14	-2.1E-14	0	-1.915116	1.915116	-1.920613	1.920613	-1E-12	4.66E-11	8.36E+77			7.775253	6.675416	6.663848	6.686983	6.52974	6.821092	8.937342	11.38353	4.503785
41										39*	11.5	0	2.65E-20	-2.65E-20	0	-2.932547	2.932547	-2.936141	2.936141	-1.63E-18	9.85E-17	8.36E+77			7.823232	7.117529	7.106507	7.128551	6.971895	7.263163	9.495868	11.89144	4.834569
42										40*	11.75	0	7.4E-28	-7.4E-28	0	-4.331082	4.331082	-4.333515	4.333515	-5.78E-26	4.47E-24	8.36E+77			7.871212	7.587008	7.576527	7.597488	7.441414	7.732601	10.07764	12.3489	5.187218
43																									7.919192	8.0849	8.074961	8.094839	7.939344	8.230455	10.67967	12.73156	5.56307
44																									7.967172	8.612081	8.602682	8.621479	8.466561	8.757601	11.2977	13.01043	5.96351
45																									8.015152	9.169186	9.160323	9.17805	9.0237	9.314673	11.92594	13.15133	6.38996
46																									8.063131	9.756533	9.748192	9.764874	9.611078	9.901988	12.55684	13.1135	6.843865
47																									8.111111	10.37402	10.36619	10.38186	10.2286	10.51945	13.18072	12.85076	7.326676
48																									8.159091	11.02105	11.01368	11.02842	10.87564	11.16645	13.78554	12.30992	7.839825
49																									8.207071	11.69634	11.6894	11.70328	11.55096	11.84172	14.35659	11.43222	8.384703
50																									8.255051	12.39788	12.39131	12.40444	12.25251	12.54324	14.87618	10.15425	8.962621
51																									8.30303	13.1227	13.11646	13.12894	12.97735	13.26805	15.32349	8.407696	9.574772
52																									8.35101	13.86677	13.8608	13.87275	13.72143	14.01211	15.67437	6.123324	10.22218
53																									8.39899	14.62483	14.61906	14.63059	14.4795	14.77016	15.90139	3.233201	10.90565
54																									8.44697	15.39019	15.3846	15.39579	15.24487	15.53552	15.97394	-0.32492	11.62569
55																									8.494949	16.15468	16.14922	16.16014	16.00936	16.3	15.85869	-4.602139	12.38247
56																									8.542929	16.90842	16.90307	16.91376	16.76311	17.05373	15.52027	-9.631302	13.17571
57																									8.590909	17.63984	17.63461	17.64508	17.49453	17.78516	14.9223	-15.41991	14.00464
58																									8.638889	18.33563	18.3305	18.34076	18.19032	18.48094	14.02887	-21.93944	14.86786
59																									8.686869	18.98078	18.97577	18.9858	18.83548	19.12609	12.80643	-29.11769	15.76331
60																									8.734848	19.55881	19.55391	19.5637	19.41351	19.7041	11.22621	-36.82746	16.68817
61																									8.782828	20.05198	20.0472	20.05676	19.90669	20.19727	9.266995	-44.87856	17.63881
62																									8.830808	20.44183	20.43715	20.4465	20.29653	20.58712	6.918307	-53.01302	18.6107
63																									8.878788	20.70968	20.70508	20.71428	20.56439	20.85497	4.183768	-60.90199	19.59845
64																									8.926768	20.83745	20.83287	20.84203	20.69216	20.98274	1.084418	-68.14883	20.59575
65																									8.974747	20.80855	20.80393	20.81318	20.66326	20.95384	-2.338329	-74.30388	21.59549
66																									9.022727	20.60891	20.60415	20.61366	20.46361	20.7542	-6.020494	-78.88063	22.5898
67																									9.070707	20.22807	20.22311	20.23303	20.08277	20.37337	-9.874584	-81.3905	23.57021
68																									9.118687	19.66035	19.65511	19.66558	19.51504	19.80566	-13.79033	-81.38077	24.52788
69																									9.166667	18.90584	18.90027	18.91141	18.76052	19.05116	-17.63757	-78.48315	25.45382
70																									9.214646	17.97126	17.96532	17.9772	17.82592	18.1166	-21.27152	-72.46497	26.3392
71																									9.262626	16.87047	16.86413	16.87682	16.72512	17.01583	-24.54053	-63.2811	27.17568
72																									9.310606	15.62458	15.61778	15.63138	15.47921	15.76996	-27.29606	-51.11224	27.95576
73																									9.358586	14.26152	14.25418	14.26886	14.11612	14.40692	-29.40427	-36.39109	28.67313
74																									9.406566	12.81505	12.807	12.82309	12.66961	12.96048	-30.7581	-19.80016	29.32295
75																									9.454545	11.32318	11.31413	11.33222	11.17768	11.46867	-31.28868	-2.239086	29.90213

goodness of fit (from TableCurve 2D)

coefficients

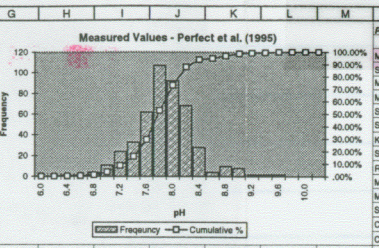
TableCurve 2D equation ref#

DeWitt

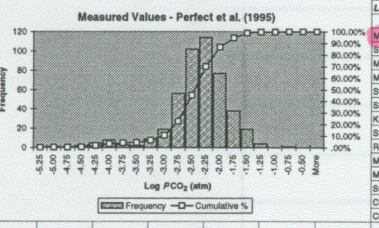
52 5/22/96 DRJ

SZ data from Measured pH, Calculated Log P_{CO_2} - Perfect et al. (1995)

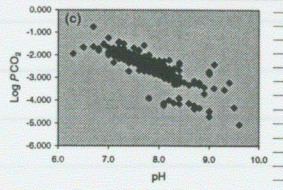
	A	B	C	D	E	F
1	**Measured Parameters (Perfect et al., 1995)**					
2	*SAMPLE*	*pH*	*Log P(CO2)*	*Bin*	*Frequency*	*Cumulative %*
3	492-SPRING	7.3	-1.963	6.0	0	,00%
4	499-WELL	8.1	-2.777	6.2	0	,00%
5	500-WELL	8.0	-2.700	6.4	1	,22%
6	501-WELL	7.7	-2.487	6.6	1	,44%
7	502-WELL	8.1	-2.688	6.8	4	1.31%
8	503-WELL	8.3	-2.971	7.0	11	3.70%
9	504-WELL	8.2	-2.890	7.2	24	8.93%
10	505-WELL	8.1	-2.714	7.4	33	16.12%
11	506-WELL	7.9	-2.483	7.6	62	29.63%
12	507-WELL	8.0	-2.593	7.8	107	52.94%
13	509-WELL	8.0	-2.650	8.0	92	72.98%
14	545-WELL	8.1	-2.722	8.2	68	87.80%
15	550-WELL	8.1	-2.665	8.4	28	93.90%
16	551-WELL	8.3	-2.915	8.6	4	94.77%
17	585-WELL	7.8	-2.483	8.8	10	96.95%
18	601-WELL	8.0	-2.550	9.0	8	98.69%
19	602-WELL	7.8	-2.353	9.2	2	99.13%
20	603-WELL	7.9	-2.559	9.4	2	99.56%
21	604-WELL	8.1	-2.643	9.6	2	100.00%
22	609-ARTESIAN WELL	7.9	-2.852	9.8	0	100.00%
23	652-WELL	8.0	-2.624	10.0	0	100.00%
24	708-WELL	8.0	-2.582	More	0	100.00%
25	709-WELL	8.0	-2.613			
26	710-WELL	7.9	-2.491	Bin	*Frequency*	*Cumulative %*
27	711-WELL	7.9	-2.453	-5.25	0	,00%
28	712-WELL	7.8	-2.434	-5.00	1	,22%
29	713-WELL	7.8	-2.565	-4.75	0	,22%
30	714-WELL	8.2	-2.814	-4.50	2	,65%
31	715-WELL	8.0	-2.659	-4.25	5	1.74%
32	716-WELL	7.8	-2.475	-4.00	8	3.48%
33	717-WELL	8.0	-2.671	-3.75	3	4.13%
34	718-WELL	8.1	-2.738	-3.50	2	4.57%
35	719-WELL	8.2	-2.820	-3.25	9	6.52%
36	723-WELL	8.1	-2.657	-3.00	19	10.65%
37	791-WELL	7.8	-2.426	-2.75	56	22.83%
38	792-WELL	8.2	-2.828	-2.50	102	45.00%
39	825-X	9.0	-2.839	-2.25	114	69.78%
40	826-X	9.3	-3.536	-2.00	77	86.52%
41	853-WELL	7.8	-2.495	-1.75	38	94.78%
42	866-SPRING	7.2	-1.860	-1.50	19	98.91%
43	888-TEST WELL	8.1	-2.271	-1.25	4	99.78%
44	889-SPRING	7.4	-2.363	-1.00	0	99.78%
45	926-WELL	8.4	-2.692	-0.75	1	100.00%
46	927-WELL	8.3	-2.609	-0.50	0	100.00%
47	943-WELL	9.0	-2.774	More	0	100.00%
48	944-WELL	9.4	-3.226			
49	945-X	9.1	-2.434			
50	947-X	9.5	-4.323			
51	948-X	9.6	-5.080			
52	960-WELL	8.3	-2.887			
53	961-WELL	8.0	-2.648			
54	971-WELL	7.2	-1.817			
55	990-X	9.0	-2.734			
56	1025-WELL	8.1	-2.709			
57	1027-WELL	7.9	-2.565			
58	1043-WELL	8.0	-2.653			
59	1057-SPRING	7.1	-1.843			
60	1062-WELL	8.0	-2.580			
61	1088-WELL	7.9	-2.227			
62	1093-WELL	8.3	-2.646			
63	1101-SPRING (HOT)	8.1	-2.746			
64	1150-SPRING	7.1	-1.691			
65	1157-SPRING	7.2	-1.732			
66	1158-SPRING	7.6	-2.113			
67	1161-SPRING	7.9	-2.380			
68	1162-SPRING	7.8	-2.291			
69	1165-SPRING	8.2	-2.743			
70	1171-SPRING	7.7	-2.233			
71	1172-SPRING	8.0	-2.643			
72	1176-SPRING	7.3	-1.993			
73	1177-POOL	7.4	-1.929			
74	1179-SPRING	7.1	-1.691			
75	1180-WELL	8.0	-2.719			
76	1191-SPRING	7.3	-1.796			
77	1194-SPRING	7.6	-2.131			
78	1199-SPRING	8.2	-2.677			
79	1200-SPRING	7.7	-2.227			
80	1205-WELL	8.4	-3.088			
81	1206-WELL	8.0	-2.494			
82	1207-WELL	7.6	-2.259			
83	1218-WELL	8.2	-2.837			
84	1219-WELL	7.8	-2.267			
85	1220-WELL	7.4	-1.884			
86	1221-WELL	6.9	-1.563			
87	1228-X	7.6	-2.095			
88	1229-X	7.6	-2.105			
89	1230-WELL	7.6	-2.196			
90	1232-SPRING	8.2	-2.758			
91	1235-WELL	7.9	-2.427			
92	1242-SEEP POOL	8.0	-2.641			
93	1243-WELL	8.4	-2.367			
94	1248-SPRING	7.5	-2.013			
95	1249-SPRING	8.0	-2.525			
96	1250-SPRING	8.1	-2.615			
97	1272-X	7.8	-2.312			
98	1274-X	7.7	-2.171			
99	1278-SPRING	7.9	-2.752			
100	1279-SPRING	8.0	-2.846			
101	1281-X	7.7	-2.080			
102	1306-SPRING	7.8	-2.234			
103	1308-SPRING	7.8	-2.231			
104	1311-SPRING	8.2	-2.894			
105	1314-SPRING	7.7	-2.440			
106	1317-WELL	7.6	-2.142			
107	1318-WELL	7.6	-2.211			
108	1319-WELL	7.3	-1.719			
109	1322-WELL	7.8	-2.196			
110	1323-WELL	7.3	-1.719			
111	1325-SPRING	7.7	-2.334			
112	1326-SPRING	8.0	-2.553			



pH-Measured	
Mean	7.832608696
Standard Erro	0.020773099
Median	7.8
Mode	7.8
Standard Dev	0.445533314
Sample Varia	0.198499934
Kurtosis	1.753896195
Skewness	0.433866949
Range	3.3
Minimum	6.3
Maximum	9.6
Sum	3603
Count	460
Confidence Le	0.040822154



Log P(CO2)-Measured	
Mean	-2.49979348
Standard Erro	0.025292171
Median	-2.449
Mode	-2.342
Standard Dev	0.542456627
Sample Varia	0.294259193
Kurtosis	3.729513105
Skewness	-1.29952424
Range	4.311
Minimum	-5.08
Maximum	-0.769
Sum	-1149.905
Count	460
Confidence Le	0.049702788



pH-pCO_2 Correlation: Measured Val.

Correlations		
	Column 1	*Column 2*
Column 1	1	
Column 2	-0.83028	1

SUMMARY OUTPUT	*Regression Statistics*
Multiple R	0.83028
R Square	0.689364
Adjusted R	0.688686
Standard E	0.302666
Observatio	460

Linear Regression Statistics

ANOVA	*df*	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	93.10898	93.10898	1016.396	2.4E-118
Residual	458	41.95599	0.091607		
Total	459	135.065			

	Coefficients	*tandard Erro*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 95.0%*	*Upper 95.0%*
Intercept	5.41821	0.248762	21.78069	1.04E-72	4.929353	5.907067	4.929353	5.907067
X Variable	-1.010902	0.031709	-31.88097	2.4E-118	-1.073215	-0.94859	-1.073215	-0.94859

RESIDUAL OUTPUT			
Observatior	*Predicted Y*	*Residuals*	*ndard Residuals*
1	-1.961378	-0.001622	-0.005365
2	-2.7701	-0.0069	-0.022822
3	-2.66901	-0.03099	-0.102502
4	-2.365739	-0.121261	-0.401079
5	-2.7701	0.0821	0.271552
6	-2.97228	0.00128	0.004235
7	-2.87119	-0.01881	-0.062215
8	-2.7701	0.0561	0.185555
9	-2.56792	0.08492	0.280877
10	-2.66901	0.07601	0.251408
11	-2.66901	0.01901	0.062876
12	-2.7701	0.0481	0.159094
13	-2.7701	0.1051	0.347626
14	-2.97228	0.05728	0.189459
15	-2.466829	-0.016171	-0.053486
16	-2.66901	0.11901	0.393633
17	-2.466829	0.113829	0.376499
18	-2.56792	0.00892	0.029502
19	-2.7701	0.1271	0.420392
20	-2.56792	-0.28408	-0.939617
21	-2.66901	0.04501	0.148873
22	-2.66901	0.08701	0.287791
23	-2.66901	0.05601	0.185256
24	-2.56792	0.07692	0.254417
25	-2.56792	0.11492	0.380105
26	-2.466829	0.032829	0.108585
27	-2.466829	-0.098171	-0.324707
28	-2.87119	0.05719	0.189161
29	-2.66901	0.01001	0.033108
30	-2.466829	-0.008171	-0.027025
31	-2.66901	-0.00199	-0.006583
32	-2.7701	0.0321	0.106173
33	-2.87119	0.05119	0.169315
34	-2.7701	0.1131	0.374086
35	-2.466829	0.040829	0.135046
36	-2.87119	0.04319	0.142855
37	-3.679912	0.840912	2.781378
38	-3.983183	0.447183	1.47909
39	-2.466829	-0.028171	-0.093177
40	-1.860288	0.000288	0.000952
41	-2.7701	0.4991	1.650809
42	-2.062468	-0.300532	-0.99403
43	-3.073371	0.381371	1.261411
44	-2.97228	0.36328	1.201576
45	-3.679912	0.905912	2.99637
46	-4.084273	0.858273	2.838801
47	-3.781002	1.347002	4.455308
48	-4.185363	-0.137637	-0.455243
49	-4.286454	-0.793546	-2.624712
50	-2.97228	0.08528	0.282071
51	-2.66901	0.02101	0.069491
52	-1.860288	0.043288	0.143178
53	-3.679912	0.945912	3.128673
54	-2.7701	0.0611	0.202093
55	-2.56792	0.00292	0.009656
56	-2.699337	0.046337	0.153262
57	-1.759198	-0.083802	-0.277183
58	-2.66901	0.08901	0.294406
59	-2.56792	0.34092	1.127616
60	-2.97228	0.32628	1.079196
61	-2.7701	0.0241	0.079713
62	-1.759198	0.068198	0.225568
63	-1.860288	0.128288	0.424321
64	-2.264649	0.151649	0.501589
65	-2.56792	0.18792	0.621557
66	-2.466829	0.175829	0.581568
67	-2.87119	0.12819	0.423999
68	-2.365739	0.132739	0.439044
69	-2.66901	0.02601	0.086029
70	-1.961378	-0.031622	-0.104592
71	-2.062468	0.133468	0.441456
72	-1.759198	0.068198	0.225568
73	-2.66901	-0.04999	-0.165346
74	-1.961378	0.165378	0.547
75	-2.264649	0.133649	0.442053
76	-2.87119	0.19419	0.642298
77	-2.365739	0.138739	0.458889
78	-3.073371	-0.014629	-0.048387
79	-2.66901	0.17501	0.578857
80	-2.224213	-0.034787	-0.115062
81	-2.891408	0.054408	0.179959
82	-2.487047	0.220047	0.727822
83	-2.062468	0.178468	0.590297
84	-1.557017	-0.005983	-0.019789
85	-2.264649	0.169649	0.561126
86	-2.264649	0.159649	0.52805
87	-2.264649	0.068649	0.227061
88	-2.87119	0.11319	0.374385

PROBABILITY OUTPUT	
Percentile	*Y*
0.108696	-5.08
0.326087	-4.732
0.543478	-4.525
0.76087	-4.478
0.978261	-4.397
1.195652	-4.355
1.413043	-4.34
1.630435	-4.323
1.847826	-4.238
2.065217	-4.228
2.282609	-4.165
2.5	-4.15
2.717391	-4.14
2.934783	-4.134
3.152174	-4.126
3.369565	-4.005
3.586957	-3.941
3.804348	-3.915
4.021739	-3.908
4.23913	-3.731
4.456522	-3.536
4.673913	-3.486
4.891304	-3.428
5.108696	-3.338
5.326087	-3.336
5.543478	-3.303
5.76087	-3.302
5.978261	-3.266
6.195652	-3.264
6.413043	-3.26
6.630435	-3.244
6.847826	-3.234
7.065217	-3.226
7.282609	-3.216
7.5	-3.185
7.717391	-3.154
7.934783	-3.104
8.152174	-3.088
8.369565	-3.08
8.586957	-3.08
8.804348	-3.071
9.021739	-3.071
9.23913	-3.07
9.456522	-3.067
9.673913	-3.067
9.891304	-3.06
10.1087	-3.024
10.32609	-3.024
10.54348	-3.021
10.76087	-2.996
10.97826	-2.993
11.19565	-2.971
11.41304	-2.962
11.63043	-2.953
11.84783	-2.952
12.06522	-2.946
12.28261	-2.915
12.5	-2.907
12.71739	-2.903
12.93478	-2.902
13.15217	-2.901
13.36957	-2.897
13.58696	-2.897
13.80435	-2.894
14.02174	-2.894
14.23913	-2.894
14.45652	-2.89
14.67391	-2.887
14.8913	-2.873
15.1087	-2.864
15.32609	-2.859
15.54348	-2.858
15.76087	-2.857
15.97826	-2.856
16.19565	-2.854
16.41304	-2.853
16.63043	-2.852
16.84783	-2.846
17.06522	-2.84
17.28261	-2.839
17.5	-2.839
17.71739	-2.838
17.93478	-2.837
18.15217	-2.837
18.36957	-2.828
18.58696	-2.82
18.80435	-2.814
19.02174	-2.813

	AH	AI
	s.d.(pH)^2	0.198499934
	s.d.(CO2)^2	0.294259193
	corr*s.d.(pH)	-0.20066407
	For Cholesky Decomposit	
	L11	0.445533314
	L21	-0.4503907
	L22	0.302336556

etc. n=460 etc.

$X_1(0,1)$ } Random numbers w/ $\bar{x} = 0$, s.d. = 1
$X_2(0,1)$ } calculated using Microsoft Excel 97
Data Analysis Tool Pak

5/22/98 (DRJ)

pH = ([s.d. pH]*X1(0,1)) + [mean pH]=(0.4455333*X1(0,1))+7.8326087

log PCO2={{corr*[s.d.pH]*[s.d.logPCO2]}/[s.d.pH]}*x1(0,1) + {sqrt{[s.d.logPCO2]^2-{{corr*[s.d.pH]*[s.d.logPCO2]}/[s.d.pH]}^2}*X2(0,1) + [mean logPCO2]=-0.45038*X1(0,1)+0.30235*X2(0,1)+-2.4997935

X1(0,1)	X2(0,1)	pH	log PCO2
-0.9659766	0.89783498	7.40223394	-1.79327825
-1.33439698	-1.78112259	7.23809039	-2.43729193
-1.84606506	0.24567612	7.01012521	-1.59406604
-1.75234618	1.28324018	7.0518801	-1.32258261
-1.24647158	0.16533704	7.27726408	-1.88840681
-0.27750048	0.77650157	7.70897299	-2.14004503
-0.41844942	-0.88395382	7.64617554	-2.5785793
0.99894805	-0.71162049	8.27767333	-3.1648593
0.15247679	-0.06242544	7.90054218	-2.5873411
-0.19005142	0.00661657	7.74793446	-2.41219565
-1.10976998	-2.2326094	7.3381692	-2.67496282
-0.00623459	0.79116717	7.82983098	-2.25778672
-0.67091605	0.88871275	7.53369324	-1.92892876
-3.563473	-0.18211267	6.24496276	-0.94989763
0.21237838	0.80960945	7.92723034	-2.3506722
-0.65320137	0.47740173	7.54158573	-2.06126165
0.56173349	0.65832296	8.08287968	-2.55375793
-0.91758466	0.80082827	7.42379416	-1.8444022
-2.67347787	-1.07872893	6.64148524	-1.62182305
-0.93698645	0.35871381	7.41515002	-1.96933118
-0.57134457	1.79474227	7.57805566	-1.69984899
1.50998858	0.13940962	8.50535891	-3.13772969
-2.14920874	0.00087994	6.8750646	-1.53154377
-0.63746825	0.77774303	7.54859536	-1.97754355
0.79012125	-0.64602091	8.18463403	-3.05097249
0.62653953	-0.37392965	8.11175293	-2.89503367
1.38013093	0.02796355	8.447503	-3.11293723
-2.04212483	-1.08477025	6.92277405	-1.90800511
-1.68852239	-0.90138883	7.08031572	-2.01182146
0.24252358	-1.32605919	7.94066103	-3.00994002
0.38222879	-0.65908353	8.00290436	-2.87121082
-1.07736014	0.12605824	7.35260886	-1.97644846
1.46556886	-0.07515382	8.48556845	-3.18259384
0.32046046	-0.43369482	7.97538451	-2.77524769
-0.52889163	-0.63045377	7.59696985	-2.45219482
0.3795958	-0.64366759	8.00173127	-2.86536415
-2.11006409	-0.36680149	6.89250485	-1.6603377
0.23300231	1.53958808	7.93641899	-2.1392618
0.01763397	0.53594249	7.84046521	-2.34570065
-0.5868128	2.89561285	7.57116404	-1.36004882
0.2927186	-0.05207994	7.96302458	-2.64737689
0.12467126	-1.86751095	7.8881539	-3.12056108
0.58517799	0.34325467	8.09332498	-2.65957378
-0.34504069	0.90702997	7.67888157	-2.07016204

	pH	Log PCO2
pH	1	
Log PCO2	-0.84998849	1

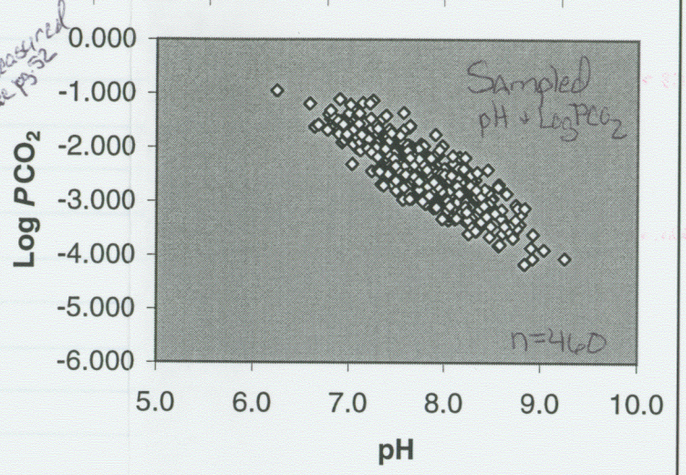
Correlation: Sampled pH + PCO_2

Sampled pH	
Mean	7.83469363
Standard Error	0.02221824
Median	7.83732914
Mode	7.84046521
Standard Dev	0.47652812
Sample Variance	0.22707904
Kurtosis	-0.06899133
Skewness	-0.11153123
Range	3.00516842
Minimum	6.24496276
Maximum	9.25013118
Sum	3603.95907
Count	460

Sampled Log PCO2	
Mean	-2.50975596
Standard Error	0.02637434
Median	-2.54201965
Mode	#N/A
Standard Dev	0.5656665
Sample Variance	0.31997859
Kurtosis	-0.07626363
Skewness	0.05296301
Range	3.20827262
Minimum	-4.15817025
Maximum	-0.94989763
Sum	-1154.48774
Count	460

L11	0.44553331
L21	-0.45039072
L22	0.30233656
mean(pH)	7.8326087
mean(logCO2	-2.49979348
s.d.(pH)^2	0.19849993
s.d.(CO2)^2	0.29425919
corr*s.d.(pH)*	-0.20066407

measured see pg 52



etc. n=460 etc.

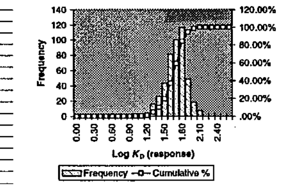
54 5/22/98 DRJ

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	*Calculate Kd response surface for each pH for all log PCO2, linear interpolation of KA (and KD) based on Correl Log PCO2*														
2	Random Generation - Based on Perfect et al. (1995			*pH-Random*		Response surface coefficients calculated by linear interpolation							Interpolated	Interpolated	Interpolated
3		Correl Log PCO2 from Random(1)						KA(mL/g)					KA(mL/g)	KD(mL/g)	Log KD
4	*pH*	*Correl Log PCO2*		Mean	7.83469363			*log PCO2 (response)*					*(response)*	*(response)*	*(response)*
5				Standard Erro	0.02221824	-5.0	-4.5	-4.0	-3.5	-3.0	-2.5	-2.0			
6	7.4	-1.793		Median	7.83732914	4.04	3.99	3.98	3.95	3.94	3.82	3.42	3.281	32.81	1.51
7	7.2	-2.437		Mode	7.84048521	3.23	3.20	3.17	3.14	3.14	3.11	2.97	3.088	30.88	1.49
8	7.0	-1.594		Standard Dev	0.47852812	2.38	2.38	2.34	2.32	2.30	2.29	2.27	2.259	22.59	1.35
9	7.1	-1.323		Sample Varia	0.22707904	2.50	2.49	2.47	2.45	2.43	2.42	2.39	2.359	23.59	1.37
10	7.3	-1.888		Kurtosis	-0.0689913	3.40	3.37	3.34	3.32	3.31	3.27	3.09	3.045	30.45	1.48
11	7.7	-2.140		Skewness	-0.1115312	6.11	6.07	6.07	6.01	5.79	5.02	3.65	3.981	39.81	1.60
12	7.8	-2.579		Range	3.00516842	5.61	5.57	5.56	5.53	5.39	4.84	3.84	4.928	49.28	1.69
13	8.3	-3.165		Minimum	6.24496276	12.74	12.58	11.81	9.83	6.49	2.63	0.67	7.587	75.87	1.88
14	7.9	-2.587		Maximum	9.25013118	7.89	7.88	7.85	7.60	6.84	5.13	2.81	5.428	54.28	1.73
15	7.7	-2.412		Sum	3603.95907	6.44	6.40	6.40	6.33	6.03	5.10	3.45	4.814	48.14	1.68
16	7.3	-2.675		Count	460	3.70	3.66	3.63	3.61	3.60	3.53	3.26	3.558	35.58	1.55
17	7.8	-2.258				7.18	7.16	7.13	7.00	6.49	5.18	3.15	4.201	42.01	1.62
18	7.5	-1.929		*Correl Log PCO2*		4.82	4.77	4.76	4.74	4.69	4.40	3.64	3.537	35.37	1.55
19	6.2	-0.950				0.88	0.88	0.90	0.91	0.91	0.92	0.90	0.866	8.66	0.94
20	7.9	-2.351		Mean	-2.509758	8.17	8.16	8.12	7.82	6.94	5.08	2.66	4.354	43.54	1.64
21	7.5	-2.061		Standard Erro	0.02637434	4.87	4.83	4.81	4.79	4.74	4.44	3.65	3.748	37.48	1.57
22	8.1	-2.554		Median	-2.5420196	10.01	10.00	9.80	9.02	7.23	4.39	1.70	4.691	46.91	1.67
23	7.4	-1.844		Mode	#N/A	4.16	4.11	4.08	4.07	4.06	3.92	3.47	3.335	33.35	1.52
24	6.6	-1.622		Standard Dev	0.5656665	1.43	1.45	1.46	1.46	1.44	1.44	1.42	1.410	14.10	1.15
25	7.4	-1.969		Sample Varia	0.31997859	4.11	4.06	4.03	4.02	4.01	3.88	3.45	3.428	34.28	1.54
26	7.6	-1.700		Kurtosis	-0.0762639	5.12	5.07	5.06	5.04	4.97	4.59	3.67	3.118	31.18	1.49
27	8.5	-3.138		Skewness	0.05296301	16.32	15.44	13.08	8.89	4.13	1.05	0.11	5.443	54.43	1.74
28	6.9	-1.532		Range	3.20827282	1.96	1.97	1.96	1.95	1.92	1.91	1.91	1.907	19.07	1.28
29	7.5	-1.978		Minimum	-4.1581702	4.92	4.87	4.86	4.84	4.79	4.47	3.66	3.620	36.20	1.56
30	8.2	-3.051		Maximum	-0.9498976	11.38	11.32	10.90	9.58	7.01	3.63	1.11	7.273	72.73	1.86
31	8.1	-2.895		Sum	-1154.4877	10.38	10.36	10.12	9.20	7.20	4.19	1.52	6.572	65.72	1.82
32	8.4	-3.113		Count	460	15.40	14.79	12.95	9.36	4.83	1.43	0.19	5.850	58.50	1.77
33	6.9	-1.908				2.10	2.10	2.09	2.07	2.05	2.04	2.03	2.031	20.31	1.31
34	7.1	-2.012				2.60	2.59	2.57	2.54	2.52	2.51	2.48	2.479	24.79	1.39
35	7.9	-3.010				8.32	8.31	8.26	7.93	6.99	5.04	2.58	7.010	70.10	1.85
36	8.0	-2.871				9.02	9.02	8.93	8.43	7.16	4.82	2.20	6.559	65.59	1.82
37	7.4	-1.976				3.77	3.73	3.70	3.68	3.68	3.60	3.30	3.287	32.87	1.52
38	8.5	-3.183				16.01	15.23	13.05	9.06	4.37	1.17	0.13	6.087	60.87	1.78
39	8.0	-2.775				8.71	8.70	8.63	8.22	7.10	4.93	2.37	6.124	61.24	1.79
40	7.6	-2.452				5.25	5.21	5.19	5.17	5.09	4.66	3.67	4.567	45.67	1.66
41	8.0	-2.865				9.01	9.01	8.91	8.43	7.16	4.82	2.21	6.532	65.32	1.82
42	6.9	-1.860				2.01	2.02	2.01	1.99	1.97	1.96	1.95	1.951	19.51	1.29
43	7.9	-2.139				8.27	8.26	8.22	7.90	6.98	5.05	2.61	3.287	32.87	1.52
44	7.8	-2.346				7.28	7.26	7.25	7.09	6.55	5.18	3.11	4.543	45.43	1.66
45	7.6	-1.380				5.07	5.03	5.01	4.99	4.92	4.56	3.67	2.525	25.25	1.40
46	8.0	-2.647				8.57	8.56	8.50	8.12	7.06	4.97	2.45	5.590	55.90	1.75
47	7.9	-3.121				7.76	7.75	7.72	7.50	6.78	5.15	2.87	6.953	69.53	1.84
48	8.1	-2.660				10.14	10.13	9.91	9.08	7.22	4.32	1.64	5.245	52.45	1.72
49	7.7	-2.070				5.87	5.83	5.82	5.78	5.60	4.94	3.60	3.791	37.91	1.58
50	7.5	-2.159				4.48	4.44	4.41	4.40	4.38	4.17	3.58	3.767	37.67	1.58
51	7.1	-1.540				2.73	2.71	2.68	2.66	2.64	2.63	2.58	2.537	25.37	1.40
52	8.0	-2.489				9.37	9.37	9.24	8.66	7.21	4.88	2.02	4.622	46.22	1.66
53	6.8	-1.477				1.78	1.79	1.79	1.78	1.75	1.74	1.74	1.733	17.33	1.24
54	7.2	-1.136				3.28	3.25	3.22	3.20	3.19	3.15	3.00	2.742	27.42	1.44
55	8.9	-4.057				20.63	15.66	8.63	2.88	0.46	0.03	0.00	9.438	94.38	1.97
56	6.8	-1.392				1.74	1.75	1.75	1.74	1.72	1.71	1.70	1.698	16.98	1.23
57	8.3	-2.847				12.65	12.49	11.76	9.82	6.53	2.89	0.69	5.414	54.14	1.73
58	7.5	-2.408				4.40	4.36	4.33	4.32	4.30	4.11	3.56	4.009	40.09	1.60
59	7.9	-2.558				8.04	8.03	8.00	7.72	6.90	5.10	2.73	5.309	53.09	1.73
60	7.8	-2.646				6.82	6.80	6.79	6.69	6.28	5.17	3.31	5.492	54.92	1.74
61	7.2	-1.793				3.23	3.20	3.17	3.15	3.14	3.11	2.97	2.914	29.14	1.46
62	8.8	-3.498				19.78	16.80	11.50	5.41	1.42	0.16	0.01	5.398	53.98	1.73
63	7.8	-2.863				7.04	7.02	7.01	6.88	6.42	5.18	3.21	6.076	60.76	1.78
64	7.8	-2.522				7.05	7.02	7.02	6.89	6.42	5.18	3.21	5.235	52.35	1.72
65	7.7	-2.533				5.95	5.91	5.91	5.86	5.67	4.97	3.59	5.016	50.16	1.70
66	7.5	-2.316				4.89	4.85	4.83	4.81	4.76	4.45	3.65	4.157	41.57	1.62
67	8.2	-2.908				11.17	11.12	10.74	9.51	7.07	3.76	1.19	6.457	64.57	1.81
68	8.1	-2.503				10.32	10.30	10.07	9.17	7.21	4.22	1.55	4.239	42.39	1.63
69	8.2	-3.339				11.65	11.58	11.09	9.65	6.93	3.47	1.01	8.774	87.74	1.94
70	8.6	-3.817				17.23	16.01	13.04	8.25	3.42	0.73	0.06	11.285	112.85	2.05
71	7.8	-2.966				6.97	6.95	6.94	6.82	6.37	5.18	3.25	5.575	55.75	1.75
72	7.6	-1.827				5.50	5.45	5.44	5.42	5.30	4.79	3.86	2.816	28.16	1.45
73	8.3	-2.888				12.56	12.41	11.70	9.81	6.57	2.94	0.72	5.755	57.55	1.76
74	8.0	-2.025				8.49	8.48	8.43	8.06	7.04	5.00	2.49	2.614	26.14	1.42
75	7.8	-2.418				7.25	7.23	7.22	7.08	6.53	5.18	3.12	4.846	48.46	1.69
76	7.6	-2.123				5.17	5.12	5.11	5.09	5.01	4.61	3.67	3.903	39.03	1.59
77	8.0	-2.709				8.97	8.97	8.88	8.40	7.15	4.84	2.23	5.795	57.95	1.76
78	7.9	-2.701				8.13	8.12	8.08	7.79	6.93	5.09	2.68	5.826	58.26	1.77
79	8.3	-3.368				13.02	12.83	11.98	9.84	6.35	2.67	0.59	8.916	89.16	1.95
80	7.1	-2.058				2.74	2.72	2.70	2.68	2.66	2.65	2.60	2.602	26.02	1.42
81	7.4	-2.062				4.03	3.99	3.96	3.94	3.93	3.82	3.42	3.471	34.71	1.54
82	8.3	-2.559				13.11	12.91	12.03	9.84	6.29	2.61	0.57	3.052	30.52	1.48
83	8.0	-2.557				8.93	8.92	8.84	8.37	7.15	4.86	2.26	5.115	51.15	1.71
84	7.8	-2.240				6.82	6.79	6.79	6.68	6.28	5.16	3.31	4.199	41.99	1.62
85	8.1	-2.806				10.49	10.47	10.21	9.25	7.19	4.13	1.47	6.003	60.03	1.78
86	7.6	-2.190				5.33	5.29	5.28	5.26	5.16	4.71	3.67	4.062	40.62	1.61
87	7.0	-1.936				2.47	2.46	2.44	2.42	2.40	2.39	2.37	2.364	23.64	1.37
88	7.4	-2.089				3.92	3.88	3.85	3.83	3.83	3.73	3.37	3.437	34.37	1.54
89	7.9	-1.764				7.95	7.94	7.91	7.65	6.88	5.12	2.77	1.665	16.65	1.22
90	7.8	-3.041				6.93	6.91	6.90	6.78	6.35	5.17	3.28	6.386	63.86	1.81
91	7.9	-2.775				7.77	7.76	7.74	7.51	6.79	5.15	2.87	6.049	60.49	1.78
92	8.2	-2.179				10.98	10.92	10.58	9.44	7.11	3.88	1.27	2.203	22.03	1.34
93	8.1	-2.973				10.72	10.69	10.39	9.35	7.18	4.01	1.37	6.988	69.88	1.84
94	7.8	-2.708				7.26	7.24	7.23	7.07	6.54	5.18	3.12	5.746	57.46	1.76
95	8.2	-2.784				11.33	11.27	10.88	9.56	7.03	3.66	1.13	5.575	55.75	1.75
96	8.2	-2.600				11.91	11.82	11.28	9.71	6.84	3.32	0.92	4.024	40.24	1.60
97	7.5	-2.562				4.92	4.87	4.85	4.84	4.78	4.48	3.66	4.503	45.03	1.65
98	7.8	-2.652				6.94	6.91	6.91	6.79	6.35	5.17	3.26	5.532	55.32	1.74
99	7.3	-1.469				3.74	3.70	3.67	3.65	3.64	3.57	3.28	2.980	29.80	1.47
100	8.1	-2.834				9.74	9.74	9.57	8.87	7.23	4.51	1.83	6.328	63.28	1.80
101	7.8	-2.456				7.31	7.29	7.28	7.12	6.56	5.18	3.09	4.999	49.99	1.70
102	8.1	-2.538				9.64	9.64	9.48	8.82	7.23	4.56	1.88	4.762	47.62	1.68
103	7.9	-2.630				7.38	7.37	7.35	7.18	6.60	5.18	3.09	5.552	55.52	1.74
104	8.1	-2.859				10.78	10.73	10.43	9.36	7.18	3.98	1.35	6.257	62.57	1.80
105	8.5	-3.649				15.77	15.06	13.02	9.19	4.55	1.27	0.18	10.331	103.31	2.01
106	7.4	-1.415				3.95	3.90	3.87	3.86	3.85	3.75	3.39	2.964	29.64	1.47
107	7.9	-2.644				7.72	7.71	7.69	7.46	6.76	5.15	2.89	5.618	56.18	1.75
108	8.0	-2.639				9.39	9.38	9.28	8.66	7.21	4.87	2.01	5.381	53.81	1.73
109	7.5	-2.333				4.55	4.51	4.48	4.47	4.44	4.22	3.60	4.013	40.13	1.60
110	8.3	-3.150				13.34	13.11	12.15	9.83	6.17	2.48	0.52	7.266	72.66	1.86
111	7.7	-2.434				5.84	5.80	5.79	5.75	5.58	4.93	3.61	4.754	47.54	1.68
112	7.6	-1.956				5.13	5.08	5.07	5.05	4.97	4.59	3.67	3.589	35.89	1.55
113	8.1	-2.703				9.85	9.84	9.66	8.93	7.23	4.46	1.76	5.589	55.89	1.75
114	6.9	-1.753				2.01	2.01	2.00	1.99	1.96	1.95	1.95	1.948	19.48	1.29
115	7.8	-2.134				6.94	6.92	6.91	6.79	6.36	5.18	3.26	3.771	37.71	1.58
116	7.2	-1.884				3.04	3.02	2.99	2.96	2.95	2.93	2.83	2.810	28.10	1.45
117	7.6	-1.594				5.55	5.51	5.50	5.47	5.34	4.81	3.65	2.712	27.12	1.43
118	8.6	-2.678				17.24	16.01	13.03	8.24	3.42	0.73	0.06	1.687	16.87	1.23
119	8.2	-2.935				10.93	10.90	10.56	9.43	7.12	3.89	1.28	6.697	66.97	1.83
120	7.7	-2.183				5.72	5.68	5.67	5.64	5.49	4.88	3.63	4.038	40.38	1.61
121	8.4	-3.314				14.19	13.84	12.56	9.73	5.66	2.02	0.35	8.217	82.17	1.91
122	8.1	-2.840				10.77	10.74	10.43	9.37	7.15	3.98	1.35	6.134	61.34	1.79
123	7.3	-2.416				3.50	3.46	3.43	3.41	3.40	3.35	3.14	3.319	33.19	1.52
124	7.7	-2.269				6.44	6.41	6.41	6.33	6.03	5.11	3.45	4.341	43.41	1.64
125	8.7	-3.062				19.67	16.61	11.63	5.57	1.50	0.17	0.01	2.012	20.12	1.30
126	7.7	-2.313				6.22	6.19	6.18	6.12	5.87	5.05	3.52	4.479	44.79	1.65
127	8.1	-2.734				10.51	10.48	10.22	9.26	7.19	4.13	1.47	5.562	55.62	1.75
128	8.2	-2.796				11.77	11.69	11.18	9.68	6.89	3.41	0.96	5.468	54.68	1.74
129	7.4	-2.513				4.22	4.18	4.15	4.14	4.12	3.97	3.50	3.979	39.79	1.60
130	7.8	-1.941				6.48	6.45	6.45	6.37	6.06	5.11	3.43	3.237	32.37	1.51
131	8.1	-2.294				10.12	10.11	9.90	9.08	7.22	4.33	1.64	3.222	32.22	1.51
132	8.0	-2.660				9.54	9.53	9.39	8.76	7.22	4.61	1.93	5.443	54.43	1.74
133	7.3	-2.095				3.48	3.44	3.41	3.39	3.38	3.33	3.13	3.170	31.70	1.50
134	8.4	-3.444				14.39	14.00	12.64	9.69	5.53	1.92	0.32	9.220	92.20	1.96

	P	Q	R	S	T	U	V
2		a	b	c	d	e	f
3	-2.0000000	-323.7345029	151.4136753	-17.3990293	-1.7541165	0.4728224	-0.0247745
4	-2.5000000	-441.4872518	226.8171288	-37.7488848	1.2089255	0.2378357	-0.0187447
5	-3.0000000	148.2265595	-173.6278793	69.4791195	-12.8694017	1.1394455	-0.0390727
6	-3.5000000	604.4445148	-474.5177627	147.2075461	-22.6668262	1.7384814	-0.0529354
7	-4.0000000	847.1361569	-620.1544804	180.5362481	-26.2031203	1.8992944	-0.0549789
8	-4.5000000	925.7298724	-652.8079408	183.1897645	-25.6433578	1.7939710	-0.0501685
9	-5.0000000	923.2318767	-632.0905621	172.1420527	-23.3803904	1.5872878	-0.0430981
10	-5.5000000	672.7843208	-452.9837012	121.1472289	-16.1548188	1.0777544	-0.0287689
11	-6.0000000	393.8474607	-256.6708687	67.3400912	-8.7498479	0.5711094	-0.0149989
12	-6.5000000	722.6946490	-436.2310889	104.2139278	-12.3723844	0.7340464	-0.0174653
13	-7.0000000	2202.1902289	-1290.5774270	299.2738666	-34.3781522	1.9602212	-0.0444424
14	no CO2	1211.3978169	-705.8275247	161.4060394	-18.1364187	1.0036927	-0.0219067

	X	Y	AA	AB
2	*KD (Response)*		*Log KD (Response)*	
4	Mean	47.1145058	Mean	1.63907544
5	Standard Erro	0.85274094	Standard Erro	0.00828859
6	Median	45.3302698	Median	1.65638826
7	Mode	#N/A	Mode	#N/A
8	Standard Dev	18.2892555	Standard Dev	0.17777053
9	Sample Varia	334.496868	Sample Varia	0.03160236
10	Kurtosis	0.93463429	Kurtosis	0.42987196
11	Skewness	0.74466404	Skewness	-0.4944108
12	Range	113.380524	Range	1.14911375
13	Minimum	8.65726225	Minimum	0.93738057
14	Maximum	122.037788	Maximum	2.08649432
15	Sum	21672.6727	Sum	753.978084
16	Count	460	Count	460

	AD	AE	AF	AG
1	0.00	*Bin*	*Frequency*	*umulative %*
2	0.10	0.00	0	.00%
3	0.20	0.10	0	.00%
4	0.30	0.20	0	.00%
5	0.40	0.30	0	.00%
6	0.50	0.40	0	.00%
7	0.60	0.50	0	.00%
8	0.70	0.60	0	.00%
9	0.80	0.70	0	.00%
10	0.90	0.80	0	.00%
11	1.00	0.90	0	.00%
12	1.10	1.00	1	.22%
13	1.20	1.10	1	.43%
14	1.30	1.20	3	1.09%
15	1.40	1.30	16	4.57%
16	1.50	1.40	26	10.22%
17	1.60	1.50	43	19.57%
18	1.70	1.60	81	37.17%
19	1.80	1.70	100	58.91%
20	1.90	1.80	116	84.13%
21	2.00	1.90	48	94.57%
22	2.10	2.00	18	98.48%
23	2.20	2.10	7	100.00%
24	2.30	2.20	0	100.00%
25	2.40	2.30	0	100.00%
26	2.50	2.40	0	100.00%
27		2.50	0	100.00%
28		More	0	100.00%



Calculating Kd using:

Sampled pH + LogPCO_2 (pg. 53)

Combination Lookup + Parameterization (pg. 51)

etc. n=460

DRJ

6/4/98
DRL

Correction of Np(V) sorption modeling in "Preliminary Fracture Sorption Module for TPA 3.2 - Letter Report" (IM 1402-871-810) (Delivered to NRC on 4/29/98) (Turner, 1998)

During preparation of "Preliminary Alluvium Sorption Module for TPA 3.2 - Letter Report" IM1402-871-830), I discovered that I had initially used the wrong equilibrium constant for the reaction:

$NpO_2^+ + CO_3^{2-} \rightleftharpoons NpO_2CO_3^-$

As stated in the text, the correct log K = 4.6. In actuality, a value of log K = 4.0 was used in the FORTRAN 77 program that I wrote to read the geochemical analyses and write the information to a file formatted for MINTEQA2, Version 3.11 input. The FORTRAN 77 code was modified to use the correct log K value (4.6):

Log K = 4.6
from Turner et al. (98)

```
....
c
c  Insert Np-Thermodynamic data from Turner et al. (1998).
c
      WRITE(9,135)
135   FORMAT('  2   4')   LogK       ΔHr
      WRITE(9,140)
140   FORMAT('5523300   -10.0000    10.5015',19X,'/npo2(oh)')
      WRITE(9,145)
145   FORMAT('5521400     4.6000    12.7951',19X,'/npo2(co3)-1')
      WRITE(9,150)
150   FORMAT('5521401     7.0000     7.1390',19X,'/npo2(co3)2-3')
      WRITE(9,155)
155   FORMAT('5521402     8.5000     6.2630',19X,'/npo2(co3)3-5')
c
....
```

DRLarry

With the corrected FORTRAN 77 code, a new set of calculations with the culled Perfect et al. (1995) data (n = 460 analyses). An example of the new input file generated for each analysis is given here:

6/4/98 (DR) MINTEQA2 input prepared based on Perfect et al. (1995) water chemistry data. Note corrected log $K_{Npo_2(co_3)^-}$ (highlighted)

```
MANSE SPRING NESESW 3-21S-54E NYE ;SampID=492-SPRING   ;ArcID=492
UTM=4000644.3 North; 599584.8 East; Date=10/28/64
23.90 MG/L   0.000  0.00000E-01
0 0 1 0 3 0 0 0 1 1 0 0 0
4   1   7
1.000E+00    9.70 0.000 0.000 81
    330  0.000E-01   -7.30 y                    /H+1
    150  0.500E+02   -2.90 y                    /Ca+2
    460  0.220E+02   -3.04 y                    /Mg+2
    500  0.470E+01   -3.69 y                    /Na+1
    410  0.900E+00   -4.64 y                    /K+1
    180  0.310E+01   -4.06 y                    /Cl-1
    732  0.270E+02   -3.55 y                    /SO4-2
    140  0.240E+03   -2.41 y                    /CO3-2
    492  0.800E+00   -4.89 y                    /NO3-1
    770  0.813E+01   -3.87 y                    /H4SiO4
    281  0.200E-01   -6.45 y                    /Fe+3
    552  2.690E-01   -6.00 y                    /npo2+
    813  0.000E-01    0.00 y                    /ADS1PSIo
    811  1.687E-05   -4.77 y                    /ADS1TYP1
    812  2.033E-05   -4.69 y                    /ADS1TYP2

  2   4
5523300   -10.0000    10.5015                   /npo2(oh)
5521400     4.6000    12.7951                   /npo2(co3)-1
5521401     7.0000     7.1390                   /npo2(co3)2-3
5521402     8.5000     6.2630                   /npo2(co3)3-5
  3   1
    330     7.3000     0.0000                   /H+1
  6   1
    813     0.0000     0.0000                   /ADS1PSIo

  2   6
5523301 npo2(oh)2-       0.0000  -22.4000   0.000   0.000-1.00 4.00 0.00   0.0000
 0.00 3   -2.000 330   1.000 552   2.000   2   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113300 >AlO-            0.0000   -9.7300   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3    1.000 811  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8113301 >AlOH2+          0.0000    8.3300   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3    1.000 811   1.000 330   1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8115520 >AlONpO2OH-      0.0000  -13.7900   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 5    1.000 811   1.000 552   1.000   2  -2.000 330  -1.000 813   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8123300 >SiO-            0.0000   -7.2000   0.000   0.000-1.00 0.00 0.00   0.0000
 0.00 3    1.000 812  -1.000 330  -1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
8125520 >SiOHNpO2+       0.0000    4.0500   0.000   0.000 1.00 0.00 0.00   0.0000
 0.00 3    1.000 812   1.000 552   1.000 813   0.000   0   0.000   0   0.000   0
   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0   0.000   0
0  0.000   0   0.000   0   0.000   0
```

compare with lines of code on pg. 55

DRDelnimm

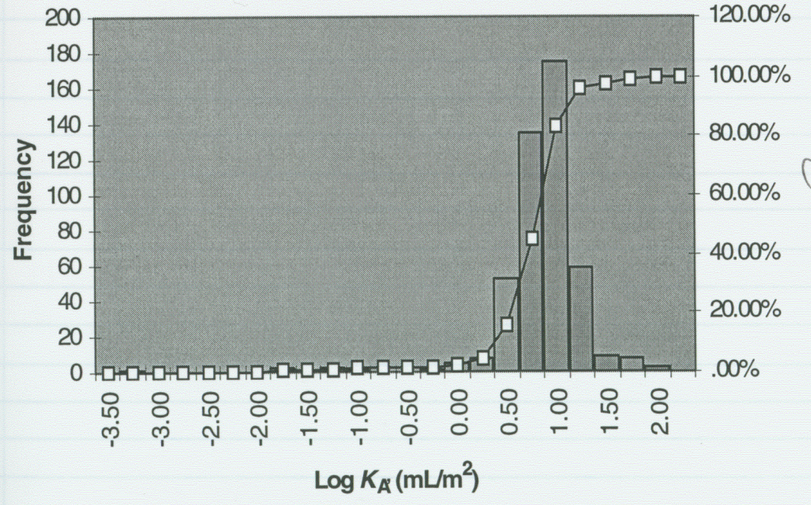
6/4/98 (DR)

The higher value for log $K_{NpO2(CO3)^-}$ (4.6 vs 4.0) results a prediction of increased carbonate complexation; all else remaining constant, the new corrected equilibrium constant will reduce the calculated sorption coefficient (K_D) relative to that originally presented in the report. This affects the descriptive statistics used for Np(V)-montmorillonite sorption coefficients and also four graphs that were included in the report. The corrected table and graphs are shown here:

Descriptive statistics of predicted Np(V)-montmorillonite sorption for groundwater chemistries reported in Perfect et al. (1995).

Np(V)-Montmorillonite	Log (K_D) (mL/g)	Log $K_{A'}$ (mL/m^2)
Mean	1.73	0.74
Standard Error	0.02	0.02
Median	1.76	0.77
Mode	1.72	0.74
Standard Deviation	0.42	0.42
Kurtosis	26.58	26.58
Skewness	-3.56	-3.56
Range	5.14	5.14
Minimum	-2.28	-3.26
Maximum	2.86	1.88
Count	460	460

highlighted values have been changed



DRDelnimm