LSNReviews

From: Osvaldo Pensado [opensado@cnwra.swri.edu]
Sent: Thursday, January 04, 2007 12:21 PM
To: James Myers; Roberto Pabalan
Subject: Original data
Attachments: brine chemistry_Pabalan.xls

These are the original data used to derive the chemistry distributions. I need something similar for each of the temperatures.

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Properties Page

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04 Jan 2007 11:20:44 -0600 (CST)
Date: Thu, 04 Jan 2007 11:20:43 -0600
From: Osvaldo Pensado <opensado@cnwra.swri.edu>
Subject: Original data
To: James Myers <jmyers@cnwra.swri.edu>,
Roberto Pabalan <rpabalan@cnwra.swri.edu>
Reply-to: opensado@cnwra.swri.edu
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3200 Coul/(m2 yr) 383.15 K

Mill annealed

Sample	Brine type	pH	Cl- molal	NO3- molal	HCO3+CO3 molal	SO4-2 molal	Ecorr(VSHE)	Ecrit(VSHE)	Ecrit(VSHE)	LC base meta	LC weld?		
SD-9_94.2 w Br&F	*Ca-Cl*	5.80	8.5028	0.014105	2.54E-09	0.00027909	444.15096	61.55	-219.04	1	1	1	
NRG-6_158.2 w Br&F	*Ca-Cl*	5.65	13.762	0.080543	3.53E-10	3.1121	450.05998	433.93	116.85	1	1	2	
UZ-14_1,277 w Br&F	*Ca-Cl*	6.55	9.1882	0.021918	5.17E-08	0.00024487	137.28442	63.66	-223.08	1	1	3	
Aq NRG-6_1290.3	Ca-Cl	6.67	24.782	11.347	4.25E-09	0.49445	135.63433	797.26	494.16	0	0	4	
Aq SD-6_471.3	Ca-Cl	7.51	9.5477	3.442	1.36E-06	1.20E-03	123.44694	842.71	567.56	0	0	5	
Aq SD-9_41.21	Ca-Cl	5.80	8.5942	0.022015	2.84E-09	2.17E-04	444.43072	68.25	-217.47	1	1	6	
Aq UZ#16_811.2	Ca-Cl	6.55	8.6148	0.016094	6.34E-08	2.64E-04	137.3164	62.60	-219.49	1	1	7	
USW SD-12/90.34	Ca-Cl	6.45	9.6024	0.024522	4.39E-08	1.39E-04	138.7237	62.89	-226.04	1	1	8	
UE-25 NRG-6/53.58	Ca-Cl	7.51	10.188	3.2687	9.49E-07	7.00E-04	123.41059	839.61	562.57	0	0	9	0.08
NRG-6_244.6 w Br&F	*Neutral*	8.70	7.0422	3.3767	6.44E-05	0.1568	106.05486	857.21	590.99	0	0	1	
UZ-14_85.2 w F-,Br-	*Neutral*	7.61	7.1472	2.5515	4.20E-06	0.0024921	121.94514	856.50	589.85	0	0	2	
Aq NRG-6_1264.5	Neutral	6.44	6.9529	3.2112	1.65E-07	0.1583	138.95922	857.81	591.97	0	0	3	
Aq SD-6_412.2	Neutral	8.16	7.4731	3.8621	1.35E-05	0.022926	113.90405	854.38	586.42	0	0	4	
Aq SD-6_443.5	Neutral	8.59	7.1121	4.1099	7.30E-05	0.16595	107.69768	856.74	590.23	0	0	5	
Aq SD-6_507.5	Neutral	6.41	6.8563	2.8299	2.22E-07	0.16642	139.40409	858.48	593.04	0	0	6	
Aq SD-9,orig	Neutral	8.28	3.9606	0.13855	3.37E-05	0.12196	112.25105	413.79	-22.13	0	1	7	
Aq UZ-14_1061.4	Neutral	8.53	6.3474	1.6313	4.63E-05	0.26293	108.57724	862.16	550.63	0	0	8	
Aq UZ-14/54.35	Neutral	5.84	14.66	2.42E-03	5.53E-09	3.28E-06	442.75593	23.60	-265.00	1	1	9	0.24
Ave J-13 with F-, Br-	*Alkaline*	10.83	4.034	1.2397	1.0929546	0.0095555	75.065188	883.75	633.86	0	0	1	
UZ-14_1,542 w Br&F	*Alkaline*	10.49	4.318	0.48815	0.873944	0.0025898	80.080875	880.51	628.63	0	0	2	
Aq NRG-7a_455.04	Alkaline	10.72	6.3966	0.3074	0.8548928	0.013187	76.76616	861.79	464.43	0	0	3	
NRG-7a_460.25	Alkaline	10.83	4.0648	0.14176	0.7190384	0.020412	75.137879	883.39	633.28	0	0	4	
Aq SD-12_455.89	Alkaline	10.92	5.5942	0.33664	1.0218108	7.50E-03	73.756748	868.17	608.70	0	0	5	
Aq SD-12_482.38	Alkaline	10.79	4.747	0.50281	0.8650252	3.09E-03	75.733946	876.00	621.34	0	0	6	
Aq SD-6_1509.9	Alkaline	10.56	6.3855	0.18069	0.2950412	0.013717	78.97597	476.50	62.23	0	1	7	
Aq UZ#16_872.8	Alkaline	10.95	4.6989	0.26828	1.2166237	0.011933	73.436907	876.48	622.12	0	0	8	
Aq UZ-14_556.53	Alkaline	10.73	5.6307	0.33508	0.4934661	0.016565	76.504472	867.86	322.15	0	0	9	
Aq WT-24_1937.0	Alkaline	10.67	5.9095	0.028781	0.3646781	0.012246	77.434918	354.68	67.63	0	1	10	
Aq NRG-6_1275.4,orig	Alkaline	8.66	7.1186	3.5161	0.000068041	0.15814	106.65529	856.69	590.16	0	0	11	0.68
										0.08	**0.23**		

Based on data on chemistry of UZ porewater samples from Yang et al. (1996, 1998, 2003)
Occurrence of
Ca-Cl brine type = 8 %
Neutral brine type = 24%
Alkaline brine type = 68 %

Sulfate makes no difference to inhibit LC
carbonate is important to inhibit LC in alkaline solutions

CDF	pH	Cl- molal	NO3- molal	HCO3+CO3 molal	SO4-2 molal
0	5.65075	3.964582333	0.002646883	3.64E-10	7.43E-06
0.041667	6.14875	4.052321471	0.023757365	3.13E-08	0.0002766
0.083333	6.43365	4.114881471	0.065582248	1.26E-07	0.001940412
0.125	6.661	4.262705588	0.112767595	3.88E-07	0.00284321
0.166667	7.51	4.455351471	0.152150875	3.76E-06	0.003547852
0.208333	8.1934	4.673877941	0.175737875	1.91223E-05	0.006011625
0.25	8.44625	4.725124265	0.22171561	0.000042079	0.00797609
0.291667	8.59605	4.852277059	0.270782529	0.000064873	0.009182185
0.333333	9.019272059	5.302040588	0.294484647	0.057978213	0.010511744
0.375	10.13880147	5.601902574	0.315032353	0.238432381	0.011896289
0.416667	10.51949265	5.624124632	0.331803176	0.324380864	0.012118729
0.458333	10.56363971	5.744885	0.335847382	0.368939468	0.012432124
0.5	10.63109559	5.907655	0.351679596	0.447916815	0.012998108
0.541667	10.68297794	6.17445	0.440134699	0.552015381	0.013400949
0.583333	10.71356618	6.386650809	0.492213838	0.690012553	0.013735847
0.625	10.72484559	6.393392426	0.50116075	0.784867848	0.015381824
0.666667	10.73586765	6.539407353	0.797847917	0.855883689	0.017173165
0.708333	10.77257353	6.810157353	1.156799875	0.862082334	0.019345589
0.75	10.80291176	6.941816176	1.804604333	0.867904136	0.042897857
0.791667	10.82738235	7.039372167	2.439542333	0.873360343	0.09373531
0.833333	10.83	7.1161365	2.7951	0.954944563	0.135556659
0.875	10.84449265	7.309606833	3.159575588	1.033267044	0.1574075
0.916667	10.89955147	8.697943	3.3562165	1.07679031	0.16422875
0.958333	10.93158088	10.044528	3.825695	1.14069451	0.18123625
1	10.94997794	24.7269	11.307475	1.216532767	3.09901175

pH	Cl- molal	NO3- mola	HCO3+CO	SO4-2 molal
1	-0.796259	-0.263593	0.907172	-0.238154
-0.796259	1	0.200434	-0.835121	0.222148
-0.263593	0.200434	1	-0.146867	0.238994
0.907172	-0.835121	-0.146867	1	-0.384214
-0.238154	0.222148	0.238994	-0.384214	1

RANK CORRELATION MATRIX (from 10,000 samples)

Direct correlation matrix (from 10,000 samples)

1	-0.668043	-0.427309	0.795657	-0.292239
-0.668043	1	0.484888	-0.617627	0.418617
-0.427309	0.484888	1	-0.409653	0.365953
0.795657	-0.617627	-0.409653	1	-0.275556
-0.292239	0.418617	0.365953	-0.275556	1

3200 Coul/(m2 yr) 383.15 K

Mill annealed

Sample	Brine type	pH	Cl- molal	NO3- molal	HCO3+CO3 molal	SO4-2 molal	Ecorr(VSHE)	Ecrit(VSHE)	Ecrit(VSHE)	LC base m	LC weld?		Brine Frequency		
SD-9_94.2 w Br&F	*Ca-Cl*	5.80	8.5028	0.014105	2.54E-09	0.00027909	444.1509559	61.55	-219.04	1	1	1			
SD-9_94.2 w Br&F	Ca-Cl	5.80	8.5028	0.014105	2.54E-09	2.79E-04	444.1509559	61.55	-219.04	1	1	2			
UZ-14_1,277 w Br&F	*Ca-Cl*	6.55	9.1882	0.021918	5.17E-08	0.00024487	137.2844159	63.66	-223.08	1	1	3			
Aq SD-6_471.3	Ca-Cl	7.51	9.5477	3.442	1.36E-06	1.20E-03	123.4469364	842.71	567.56	0	0	4			
Aq SD-6_471.3	Ca-Cl	7.51	9.5477	3.442	1.36E-06	1.20E-03	123.4469364	842.71	567.56	0	0	5			
Aq SD-9_41.21	Ca-Cl	5.80	8.5942	0.022015	2.84E-09	2.17E-04	444.4307179	68.25	-217.47	1	1	6			
Aq UZ#16_811.2	Ca-Cl	6.55	8.6148	0.016094	6.34E-08	2.64E-04	137.3164	62.60	-219.49	1	1	7			
USW SD-12/90.34	Ca-Cl	6.45	9.6024	0.024522	4.39E-08	1.39E-04	138.7236999	62.89	-226.04	1	1	8			
UE-25 NRG-6/53.58	Ca-Cl	7.51	10.188	3.2687	9.49E-07	7.00E-04	123.4105908	839.61	562.57	0	0	9	0.08	0.6666667	0.66666667
NRG-6_244.6 w Br&F	*Neutral*	8.70	7.0422	3.3767	6.44E-05	0.1568	106.0548616	857.21	590.99	0	0	1			
UZ-14_85.2 w F-,Br-	*Neutral*	7.61	7.1472	2.5515	4.20E-06	0.0024921	121.9451381	856.50	589.85	0	0	2			
Aq NRG-6_1264.5	Neutral	6.44	6.9529	3.2112	1.65E-07	0.1583	138.959219	857.81	591.97	0	0	3			
Aq SD-6_412.2	Neutral	8.16	7.4731	3.8621	1.35E-05	0.022926	113.9040476	854.38	586.42	0	0	4			
Aq SD-6_443.5	Neutral	8.59	7.1121	4.1099	7.30E-05	0.16595	107.6976807	856.74	590.23	0	0	5			
Aq SD-6_507.5	Neutral	6.41	6.8563	2.8299	2.22E-07	0.16642	139.4040886	858.48	593.04	0	0	6			
Aq SD-9,orig	Neutral	8.28	3.9606	0.13855	3.37E-05	0.12196	112.2510518	413.79	-22.13	0	1	7			
Aq UZ-14_1061.4	Neutral	8.53	6.3474	1.6313	4.63E-05	0.26293	108.5772431	862.16	550.63	0	0	8			
Aq UZ-14/54.35	Neutral	5.84	7.4731	2.42E-03	5.53E-09	3.28E-06	442.7559263	56.97	-212.72	1	1	9	0.24	0.1111111	0.22222222
Ave J-13 with F-, Br-	*Alkaline*	10.83	4.034	1.2397	1.0929546	0.0095555	75.06518804	883.75	633.86	0	0	1			
UZ-14_1,542 w Br&F	*Alkaline*	10.49	4.318	0.48815	0.873944	0.0025898	80.08087456	880.51	628.63	0	0	2			
Aq NRG-7a_455.04	Alkaline	10.72	6.3966	0.3074	0.8548928	0.013187	76.76615999	861.79	464.43	0	0	3			
NRG-7a_460.25	Alkaline	10.83	4.0648	0.14176	0.7190384	0.020412	75.13787915	883.39	633.28	0	0	4			
Aq SD-12_455.89	Alkaline	10.92	5.5942	0.33664	1.0218108	7.50E-03	73.75674808	868.17	608.70	0	0	5			
Aq SD-12_482.38	Alkaline	10.79	4.747	0.50281	0.8650252	3.09E-03	75.73394624	876.00	621.34	0	0	6			
Aq SD-6_1509.9	Alkaline	10.56	6.3855	0.18069	0.2950412	0.013717	78.97596971	476.50	62.23	0	1	7			
Aq UZ#16_872.8	Alkaline	10.95	4.6989	0.26828	1.2166237	0.011933	73.4369072	876.48	622.12	0	0	8			
Aq UZ-14_556.53	Alkaline	10.73	5.6307	0.33508	0.4934661	0.016565	76.504472	867.86	322.15	0	0	9			
Aq WT-24_1937.0	Alkaline	10.67	5.9095	0.028781	0.3646781	0.012246	77.4349182	354.68	67.63	0	1	10			
Aq NRG-6_1275.4,orig	Alkaline	8.66	7.1186	3.5161	0.000068041	0.15814	106.6552902	856.69	590.16	0	0	11	0.68	0	0.18181818
										0.08	**0.23**				

Based on data on chemistry of UZ porewater samples from Yang et al. (1996, 1998, 2003)
Occurrence of
Ca-Cl brine type = 8 %
Neutral brine type = 24%
Alkaline brine type = 68 %

[Cl] outliers were removed to avoid extrapolation far beyond the range of validity of the corrosion equations. Ouliers were removed by replacing for conditions that would yield similar expected corrosion mode (general or localized); i.e., ranks were preserved. Removal of the outliers makes no difference in the prediction of the onset of localized corrosion.

Sulfate makes no difference to inhibit LC
carbonate is important to inhibit LC in alkaline solutions

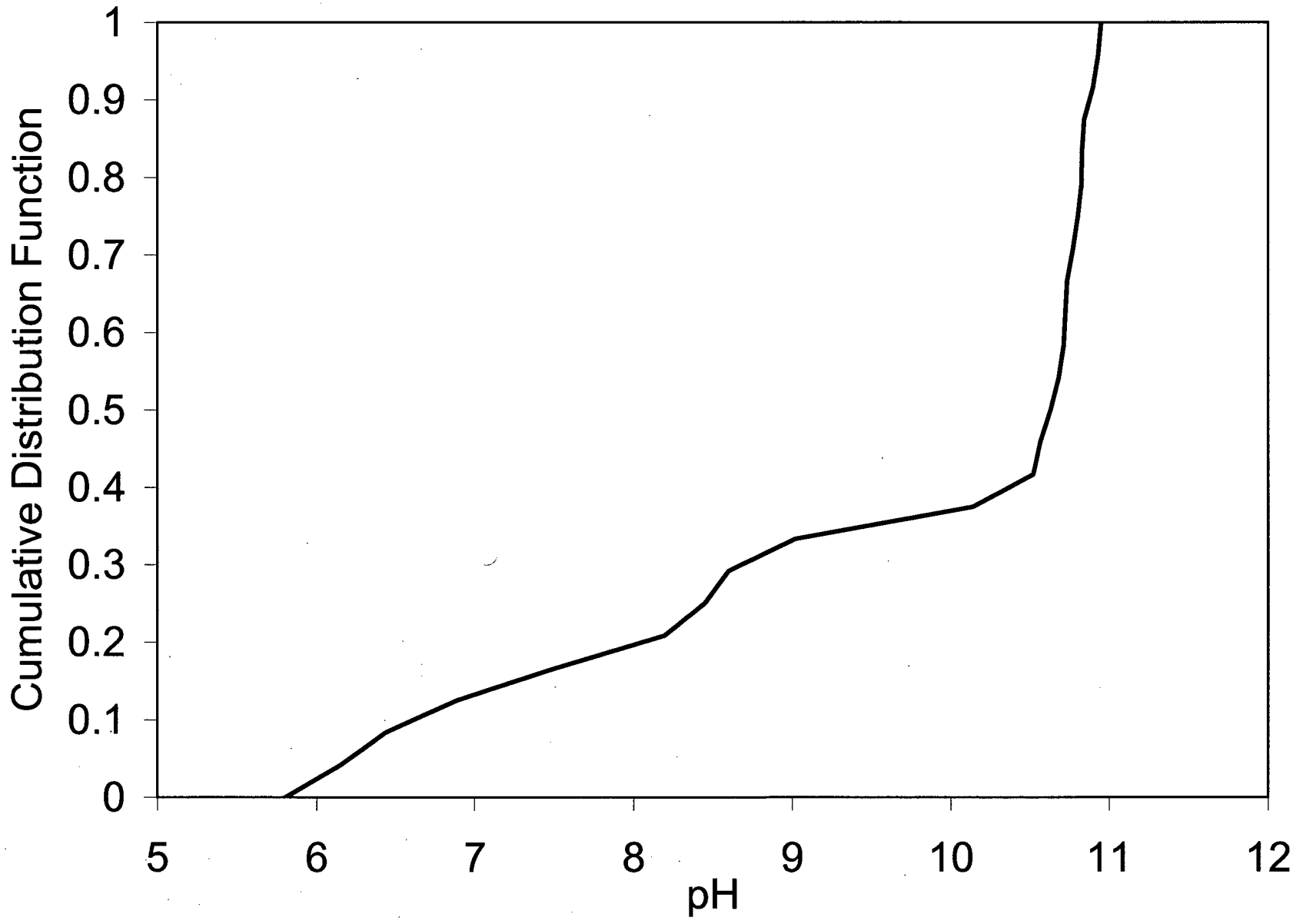
CDF	pH	Cl- molal	NO3- molal	HCO3+CO3 m	SO4-2 molal	CDF
0	5.8	3.964578	0.00264688	2.54E-09	7.43E-06	0
0.04166667	6.14875	4.05232147	0.0219893	4.69E-08	0.00027653	0.04166667
0.083	6.434	4.115	0.062	1.69085E-07	0.0011675	0.083
0.125	6.887	4.263	0.112	9.1815E-07	0.00269756	0.125
0.167	7.510	4.455	0.152	3.75579E-06	0.00300136	0.167
0.208	8.193	4.674	0.176	1.91223E-05	0.00483779	0.208
0.250	8.446	4.725	0.221	0.000042079	0.00729571	0.250
0.292	8.596	4.852	0.271	0.000064873	0.00860785	0.292
0.333	9.019	5.301	0.294	0.058	0.00985444	0.333
0.375	10.139	5.602	0.315	0.238	0.011	0.375
0.417	10.519	5.624	0.332	0.324	0.012	0.417
0.458	10.564	5.745	0.336	0.369	0.012	0.458
0.500	10.631	5.907	0.351	0.448	0.013	0.500
0.542	10.683	6.174	0.440	0.552	0.013	0.542
0.583	10.714	6.387	0.492	0.690	0.014	0.583
0.625	10.725	6.393	0.501	0.785	0.015	0.625
0.667	10.736	6.538	0.796	0.856	0.016	0.667
0.708	10.773	6.810	1.156	0.862	0.018	0.708
0.750	10.803	6.942	1.804	0.868	0.021	0.750
0.792	10.827	7.039	2.440	0.873	0.071	0.792
0.833	10.830	7.116	2.795	0.955	0.123	0.833
0.875	10.844	7.310	3.160	1.033	0.154	0.875
0.917	10.900	7.473	3.356	1.077	0.160	0.917
0.958	10.932	9.088	3.672	1.141	0.166	0.958
1.000	10.950	10.185	4.109	1.217	0.263	1.000

pH	Cl- molal	NO3- molal	HCO3+CO3 r	SO4-2 molal
1	-0.78134001	-0.2218284	0.88309778	-0.08984131
-0.78134001	1	0.17888666	-0.82166621	0.00576777
-0.2218284	0.17888666	1	-0.24372211	0.26664207
0.88309778	-0.82166621	-0.24372211	1	-0.07574479
-0.08984131	0.00576777	0.26664207	-0.07574479	1

RANK CORRELATION MATRIX (from 10,000 samples)

Direct correlation matrix (from 10,000 samples)

1	-0.74574956	-0.43087176	0.79644274	-0.41065995
-0.74574956	1	0.29296836	-0.7645445	0.17542512
-0.43087176	0.29296836	1	-0.46214391	0.43667137
0.79644274	-0.7645445	-0.46214391	1	-0.41827622
-0.41065995	0.17542512	0.43667137	-0.41827622	1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0.4
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0.2
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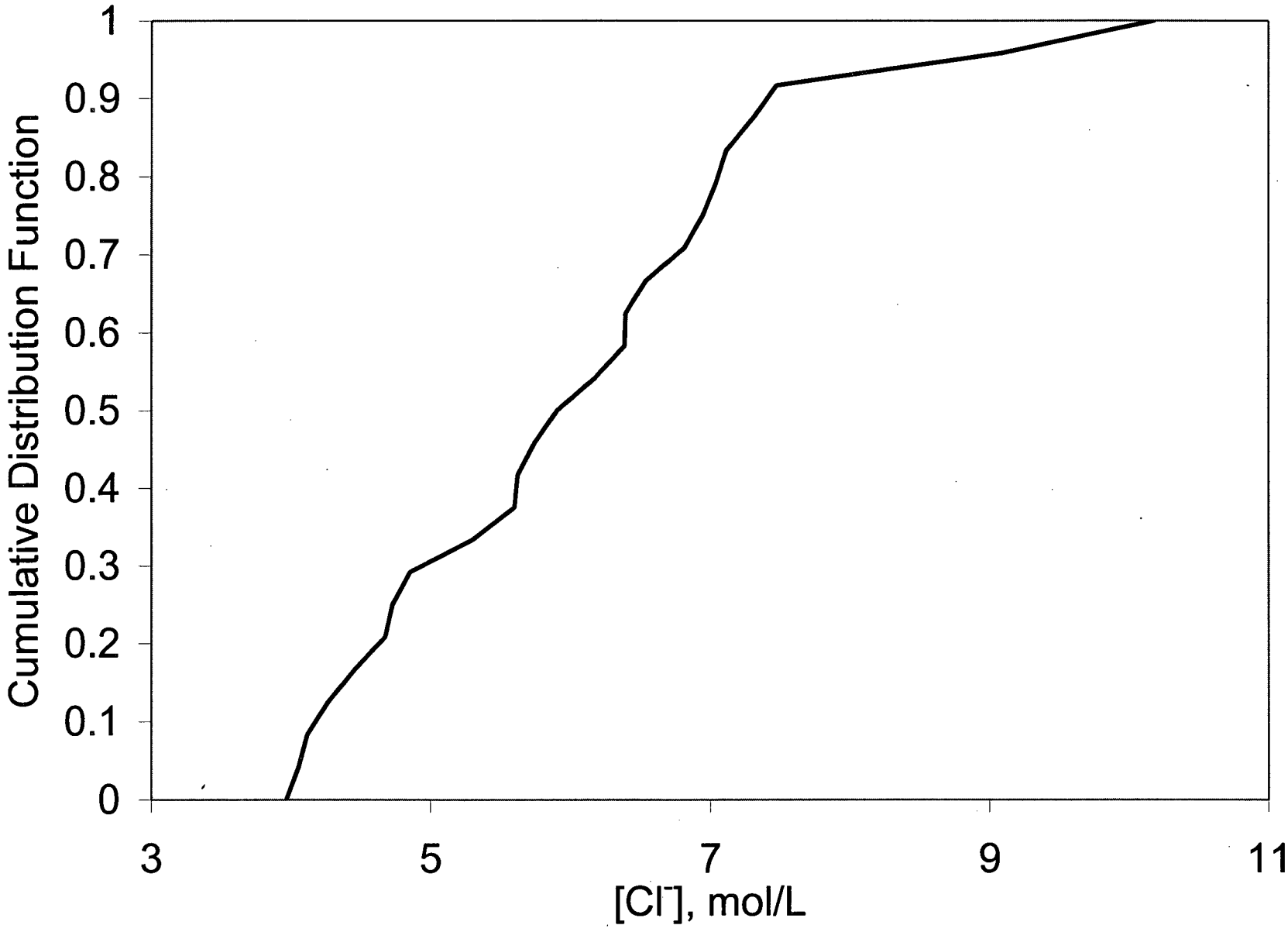
0
5
6
7
8
9
10
11
12
pH


Cumulative Distribution Function
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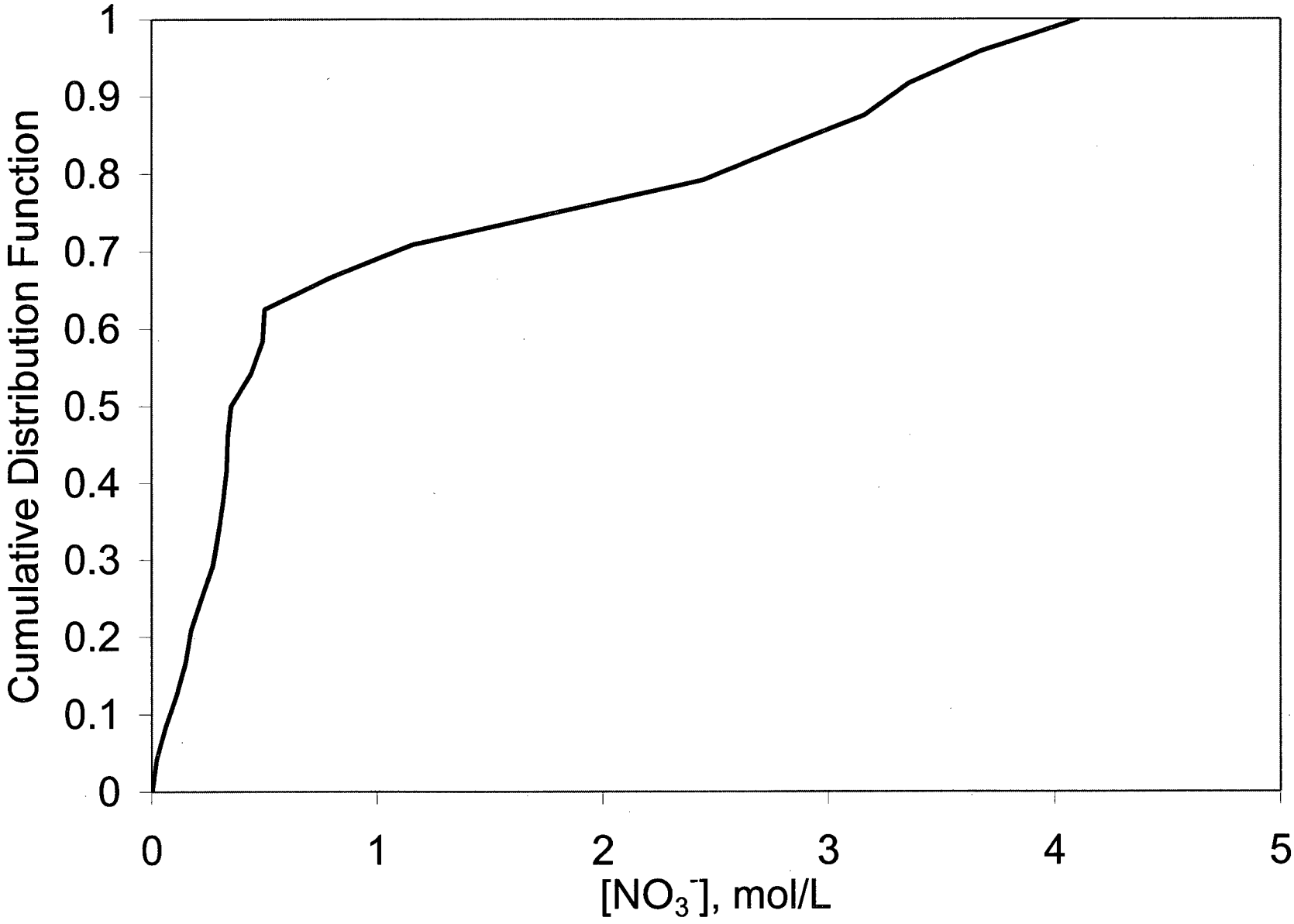
[Cl⁻], mol/L


Cumulative Distribution Function
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4
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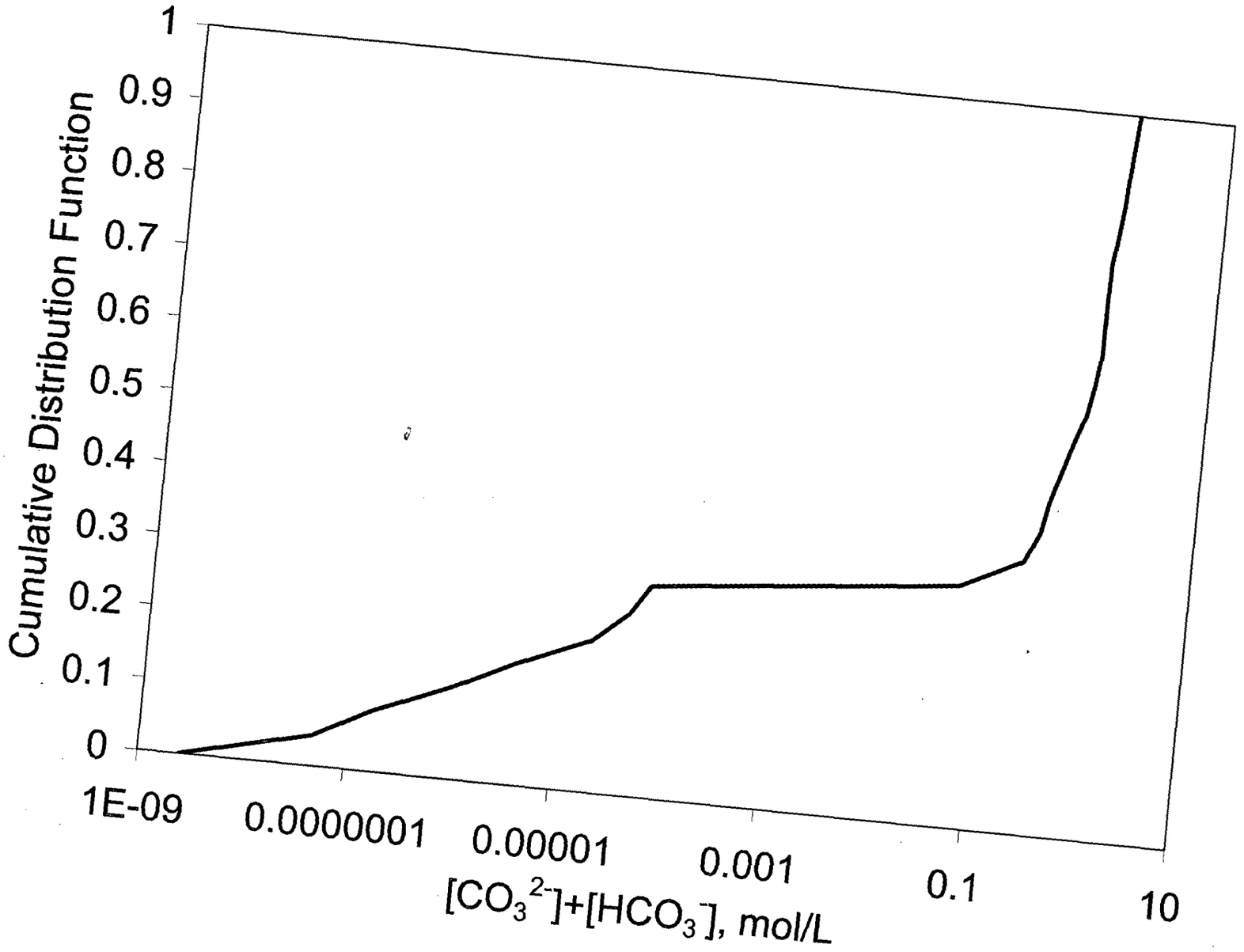
[NO3-], mol/L


Cumulative Distribution Function
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0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
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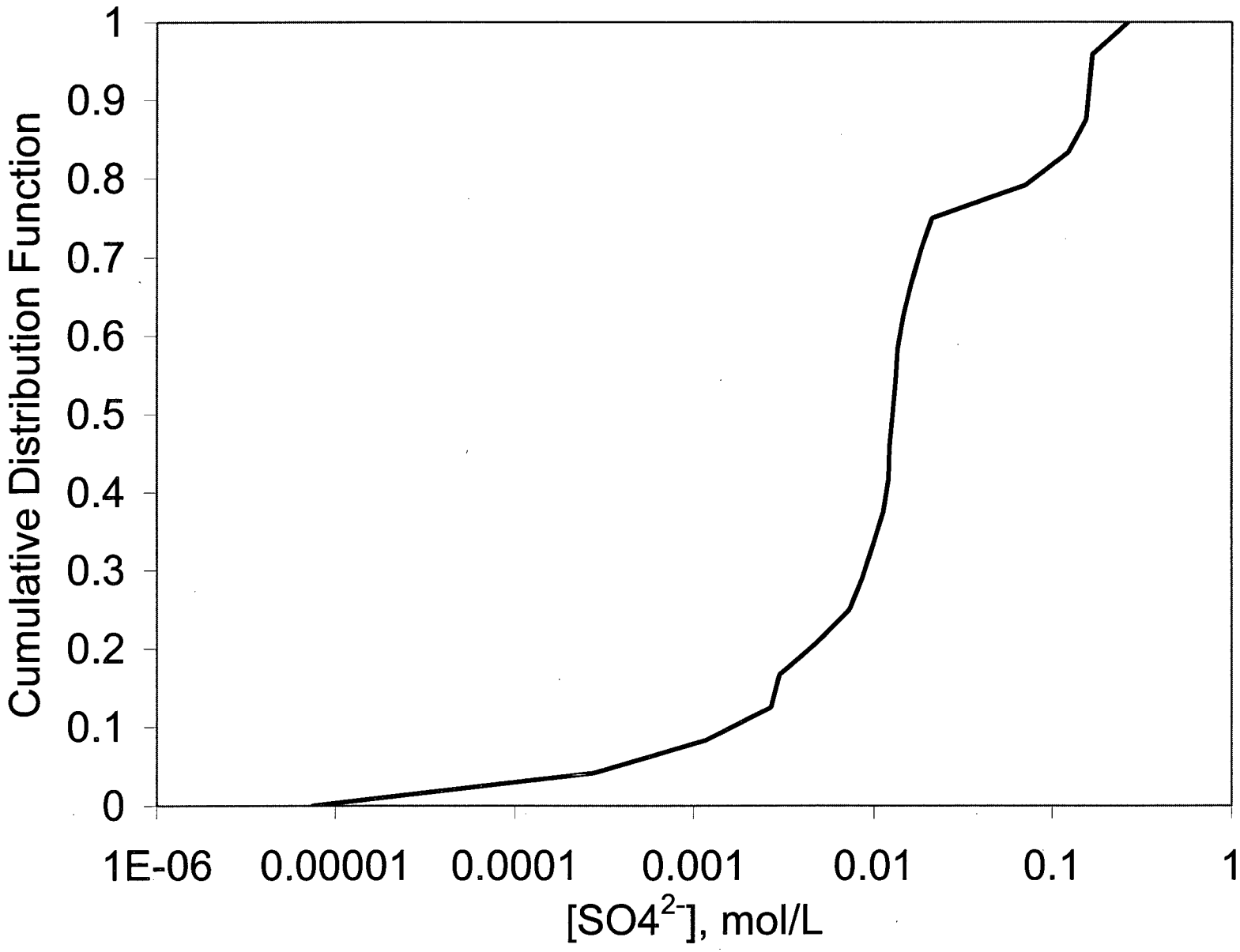
0.0000001
0.00001
0.001
0.1
10
[CO3 2-]+[HCO3 -], mol/L


Cumulative Distribution Function
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
1E-06
0.00001
0.0001
0.001
0.01
0.1
1
[SO4^{2-}], mol/L