

1-Jun-05 FPB

Initial Entry: This notebook will be used to document analyses and calculations to support development and review of RT-related parameters used in the TPA code. Work is conducted to support NRC-related work in preparation of a review of a potential license application from the DOE for the potential repository at Yucca Mountain, Nevada. This work will support both the RTUZ and RTSZ ISIs, even though the project number listed is for the RTSZ ISI. F. Paul Bertetti (initials - FPB) will conduct the tasks documented in this notebook. No particular special training or qualifications are required to perform this work.

An initial effort will be made to evaluate available geochemistry data from the Yucca Mountain region to determine appropriate range and distribution types for pH and CO₂, to be sampled within the TPA Version 5.0 code. Data are plotted and statistically analyzed in an effort to characterize trends and determine the best representation of the data within TPA. Several software packages may be used in the analyses including SYSTAT Version 11, GoldSim Version 8.02, Excel Version 2002, TableCurve 2D Version 4.07 and others as indicated within this notebook. None of the software packages mentioned thus far are controlled under TOP-018, but all are commercially available and sufficient information will be provided in this notebook to reproduce or recreate any calculations or analyses as necessary. Input and output files, if not included in this notebook explicitly, will be referenced accordingly, and electronic copies of these files will be provided with the hard copy of this notebook when completed.

Useful references:

AISN Software Inc. "TableCurve Version 4.07." Chicago, Illinois: AISN Software Inc., distributed by SPSS, Inc. 1996.

Golder Technology Group. "Software Code: GoldSim (registered trademark of Golder Associates Inc.) Version 01." Redmond, Washington: Golder Associates Inc., Golder Technology Group. 2003.

Microsoft Corporation. "Microsoft Excel 2002." Redmond, Washington: Microsoft Corporation. 2001.

Systat Software. "SYSTAT Version 11." Port Richmond, California: Systat Software. 2004.

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Below is a table of general descriptive statistics for several sets of data from the YM region. The Turner_pH and Turner_CO2 labels refer to data analyzed by Turner and Pabalan (1999) [Turner, D.R. and R.T. Pabalan. "Abstraction of Mechanistic Sorption Model Results for Performance Assessment Calculations at Yucca Mountain, Nevada." Waste Management. Vol. 19. pp. 375-388. 1999] and selected from the Perfect et al. (1995) [Perfect, D.L., C.C. Faunt, W.C. Steinkampf, and A.K. Turner. Hydrochemical Database for the Death Valley Region, California and Nevada. USGS Open-File Report 94-305. Denver, CO: United States Geological Survey. 1995] database. The YMREG_PH and YMREG_CO2 include data from DOE's Geochemistry AMR (2004) [Bechtel SAIC Company, LLC. "Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing, and Recharge at Yucca Mountain, Nevada." ANL-NBS-HS-000021, Rev 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004] and additional YM region data collected by CNWRA and Nye County as part of our sampling of EWDP wells in Fortymile Wash and the surrounding areas. The CNWRA data is summarized in Bertetti et al. (2004) [Bertetti, F. P., J. Prikryl, and B. Werling. Development of Updated Total-System Performance Assessment Parameter Distributions for Radionuclide Transport in the Saturated Zone. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2004.] The SITE_PH and SITE_CO2 data are a subset of the YMREG data with inclusion of wells or sampling points contained within the DOE site-scale model boundary for YM TSPA simulations. The limits of the site-scale boundary can be found in [Bechtel SAIC Company, LLC. Site-Scale Saturated Zone Flow Model. MDL-NBS-HS-000011. Rev 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003] and other DOE documents such as the Geochemistry AMR listed earlier.

SYSTAT Rectangular file D:\Systat_data\YM_Chem.syd,
 created Wed Mar 16, 2005 at 15:26:26, contains variables:

GROUP\$ VAR00007	ALL_PH TURNER_PH	ALL_CO2 TURNER_CO2	VAR00004 VAR00010	YMREG_PH SITE_PH	YMREG_CO2 SITE_CO2	
	YMREG_PH	YMREG_CO2	TURNER_PH	TURNER_CO2	SITE_PH	SITE_CO2
N of cases	226	221	460	460	107	107
Minimum	6.600	-4.530	6.300	-5.080	6.600	-4.530
Maximum	9.500	-0.580	9.600	-0.769	9.500	-0.580
Range	2.900	3.950	3.300	4.311	2.900	3.950
Sum	1782.440	-572.240	3603.300	-1149.905	841.840	-276.630
Median	7.900	-2.590	7.800	-2.449	7.800	-2.590
Mean	7.887	-2.589	7.833	-2.500	7.868	-2.585
95% CI Upper	7.955	-2.509	7.874	-2.450	7.983	-2.457
95% CI Lower	7.818	-2.670	7.792	-2.549	7.752	-2.714
Std. Error	0.035	0.041	0.021	0.025	0.058	0.065
Standard Dev	0.523	0.606	0.446	0.542	0.602	0.672
Variance	0.274	0.367	0.198	0.294	0.363	0.452
C.V.	0.066	-0.234	0.057	-0.217	0.077	-0.260
Skewness(G1)	0.268	0.075	0.431	-1.300	0.199	0.331
SE Skewness	0.162	0.164	0.114	0.114	0.234	0.234
Kurtosis(G2)	0.254	0.829	1.754	3.730	-0.403	0.670
SE Kurtosis	0.322	0.326	0.227	0.227	0.463	0.463
SW Statistic	0.990	0.990	0.966	0.908	0.988	0.986
SW P-Value	0.110	0.150	0.000	0.000	0.476	0.337

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GROUP\$ VAR00007	ALL_PH TURNER_PH	ALL_CO2 TURNER_CO2	VAR00004 VAR00010	YMREG_PH SITE_PH	YMREG_CO2 SITE_CO2
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Effects coding used for categorical variables in model.

Categorical values encountered during processing are:

GROUP\$ (3 levels)

Turner, YMALL, YMSUB

8 case(s) deleted due to missing data.

Number of cases processed: 788

Dependent variable means

	ALL PH	ALL CO2
	7.852	-2.537

-1
Estimates of effects $B = (X'X)^{-1} X'Y$

		ALL PH	ALL CO2
CONSTANT		7.861	-2.558
GROUP\$	Turner	-0.028	0.058
GROUP\$	YMALL	0.021	-0.031

Standardized estimates of effects

		ALL PH	ALL CO2
CONSTANT		0.000	0.000
GROUP\$	Turner	-0.041	0.072
GROUP\$	YMALL	0.027	-0.034

Total sum of product matrix

	ALL PH	ALL CO2
ALL PH	191.119	
ALL CO2	-200.930	265.194

Residual sum of product matrix $E'E = Y'Y - Y'XB$

	ALL PH	ALL CO2
ALL PH	190.725	
ALL CO2	-200.175	263.702

Residual covariance matrix S

Y.X

	ALL PH	ALL CO2
ALL PH	0.243	
ALL CO2	-0.255	0.336

Residual correlation matrix R

Y.X

	ALL PH	ALL CO2
ALL PH	1.000	
ALL CO2	-0.893	1.000

Least squares means

GROUP\$ =Turner N of Cases = 460.000

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	ALL PH	ALL CO2
LS Mean	7.833	-2.500
SE	0.023	0.027

GROUP\$ =YMALL N of Cases = 221.000

	ALL PH	ALL CO2
LS Mean	7.883	-2.589
SE	0.033	0.039

GROUP\$ =YMSUB N of Cases = 107.000

	ALL PH	ALL CO2
LS Mean	7.868	-2.585
SE	0.048	0.056

Test for effect called: CONSTANT

Null hypothesis contrast AB

	ALL PH	ALL CO2
	7.861	-2.558

Inverse contrast $A(X'X)^{-1}A'$

0.002

Hypothesis sum of product matrix $H = B'A'(A(X'X)^{-1}A')^{-1}AB$

	ALL PH	ALL CO2
ALL PH	34664.604	
ALL CO2	-11280.427	3670.835

Error sum of product matrix $G = E'E$

	ALL PH	ALL CO2
ALL PH	190.725	
ALL CO2	-200.175	263.702

Univariate F Tests

Source	SS	df	MS	F	P
ALL PH	34664.604	1	34664.604	142675.126	0.000
Error	190.725	785	0.243		
ALL CO2	3670.835	1	3670.835	10927.506	0.000
Error	263.702	785	0.336		

Multivariate Test Statistics

Statistic	Value	F-Statistic	df	Prob
Wilks' Lambda	0.002	204161.978	2, 784	0.000
Pillai Trace	0.998	204161.978	2, 784	0.000
Hotelling-Lawley Trace	520.821	204161.978	2, 784	0.000

Test of Residual Roots

Roots	Chi-Square Statistic	df
1 through 1	4912.000	2

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Canonical correlations

0.999

Dependent variable canonical coefficients standardized
by conditional (within groups) standard deviations

ALL_PH	2.188
ALL_CO2	1.790

Canonical loadings (correlations between conditional
dependent variables and dependent canonical factors)

ALL_PH	0.591
ALL_CO2	-0.163

Test for effect called: GROUP\$

Null hypothesis contrast AB

	ALL_PH	ALL_CO2
1	-0.028	0.058
2	0.021	-0.031

Inverse contrast $A(X'X)^{-1}A'$

	1	2
1	0.003	
2	-0.000	0.003

Hypothesis sum of product matrix $H = B'A'(A(X'X)^{-1}A')^{-1}AB$

	ALL_PH	ALL_CO2
ALL_PH	0.394	
ALL_CO2	-0.755	1.491

Error sum of product matrix $G = E'E$

	ALL_PH	ALL_CO2
ALL_PH	190.725	
ALL_CO2	-200.175	263.702

Univariate F Tests

Source	SS	df	MS	F	P
ALL_PH	0.394	2	0.197	0.810	0.445
Error	190.725	785	0.243		
ALL_CO2	1.491	2	0.746	2.220	0.109
Error	263.702	785	0.336		

Multivariate Test Statistics

Statistic	Value	F-Statistic	df	Prob
Wilks' Lambda	0.992	1.649	4, 1568	0.160
Pillai Trace	0.008	1.648	4, 1570	0.160
Hotelling-Lawley Trace	0.008	1.650	4, 1566	0.159

THETA	S	M	N	Prob
0.008	2	-0.5	391.0	0.128

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Test of Residual Roots

	Roots	Chi-Square	Statistic	df
1 through	2	6.585		4
2 through	2	0.166		1

Canonical correlations

	1	2
	0.090	0.015

Dependent variable canonical coefficients standardized
 by conditional (within groups) standard deviations

	1	2
ALL_PH	1.254	1.829
ALL_CO2	1.944	1.067

Canonical loadings (correlations between conditional
 dependent variables and dependent canonical factors)

	1	2
ALL_PH	-0.481	0.877
ALL_CO2	0.825	-0.566

SYSTAT Rectangular file D:\Systat_data\YM_Chem.syd,
 created Wed Mar 16, 2005 at 14:26:26, contains variables:

GROUP\$	ALL_PH	ALL_CO2	VAR00004	YMREG_PH	YMREG_CO2
VAR00007	TURNER_PH	TURNER_CO2	VAR00010	SITE_PH	SITE_CO2

Variable Name: YMREG_PH

Distribution: Normal

Estimated: Location or mean (μ) = 7.886903 Scale or SD (σ) = 0.522006

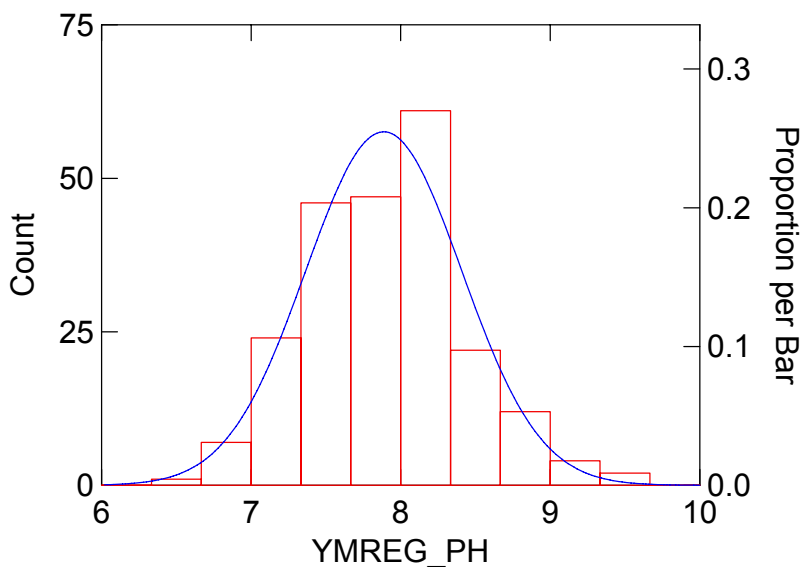
Estimation of parameter(s): Maximum likelihood method.

Test Results:

LimitL	LimitU	Observed	Expected
.	6.890	6.0	6.347
6.890	7.180	8.0	13.504
7.180	7.470	30.0	28.117
7.470	7.760	55.0	43.328
7.760	8.050	45.0	49.423
8.050	8.340	42.0	41.731
8.340	8.630	22.0	26.083
8.630	8.920	11.0	12.065
8.920	.	7.0	5.402
		226.000	226.000

Chi-square test statistic = 7.136264 df = 6 p-value = 0.308429

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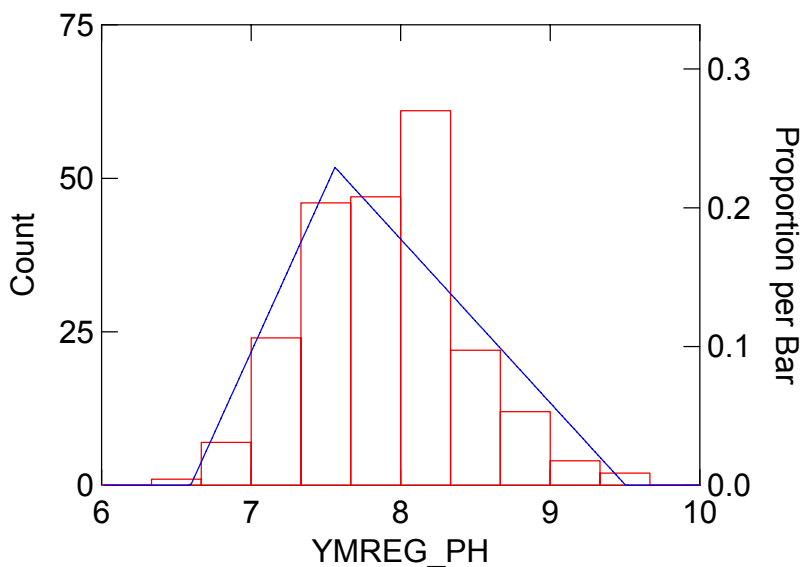
Kolmogorov-Smirnov test statistic = 0.069049 Lilliefors Probability (2-tail) = 0.010874
 Shapiro-Wilk test statistic for normality = 0.989757 p-value = 0.109584

Variable Name: YMREG_PH
 Distribution: Triangular
 Estimated: Low (a)=6.595575 High (b) = 9.504425 Mode (c) = 7.560708
 Estimation of parameter(s): Modified maximum likelihood and moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.890	6.0	6.978
6.890	7.180	8.0	20.517
7.180	7.470	30.0	34.057
7.470	7.760	55.0	42.813
7.760	8.050	45.0	37.081
8.050	8.340	42.0	30.357
8.340	8.630	22.0	23.634
8.630	8.920	11.0	16.911
8.920	.	7.0	13.652
		226.000	226.000

Chi-square test statistic = 23.303340 df = 5 p-value = 0.000295

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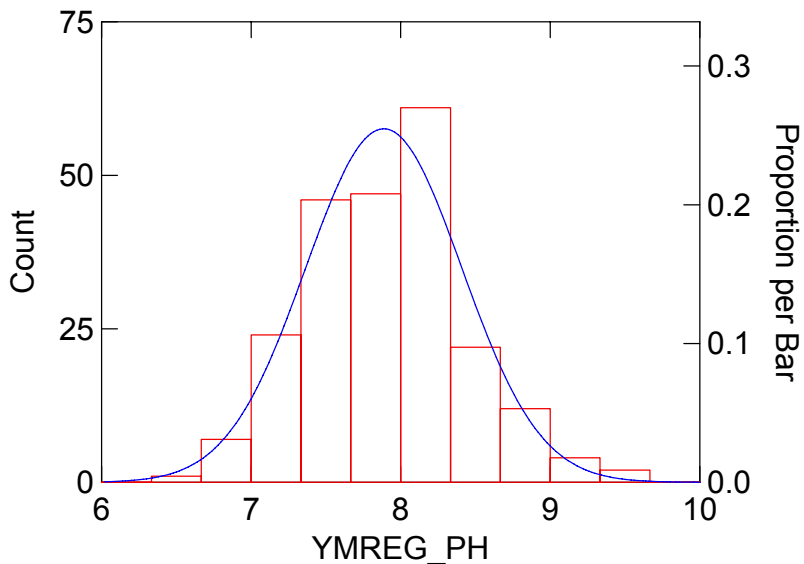
WARNING
 One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.101897 p-value(2-tail) = 0.018316

Variable Name: YMREG_PH
 Distribution: Gamma
 Estimated: Shape (alpha) = 228.276783 Scale (beta) = 0.034550
 Estimation of parameter(s): Method of moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.890	6.0	5.463
6.890	7.180	8.0	13.658
7.180	7.470	30.0	29.344
7.470	7.760	55.0	44.651
7.760	8.050	45.0	49.309
8.050	8.340	42.0	40.393
8.340	8.630	22.0	25.036
8.630	8.920	11.0	11.955
8.920	.	7.0	6.191
		226.000	226.000

Chi-square test statistic = 5.800409 df = 6 p-value = 0.445916

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WARNING

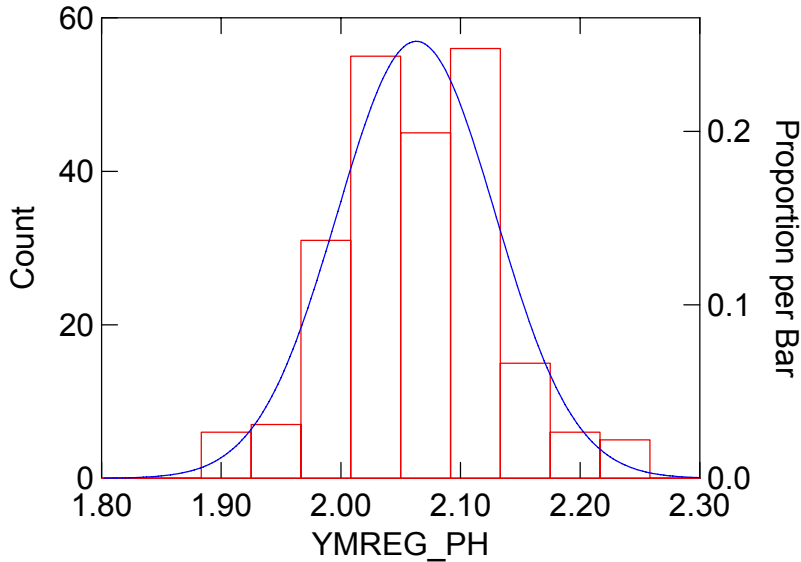
One or more parameters of distribution are estimated.
Significance of K-S test computed on this distribution is suspect.
Kolmogorov-Smirnov test statistic = 0.061842 p-value(2-tail) = 0.353054

Variable Name: YMREG_PH
Distribution: Lognormal
Estimated: Location (mu) = 2.063024 Scale (sigma) = 0.065982
Estimation of parameter(s): Maximum likelihood method.
Test Results:
Log transformation is used on data.

LimitL	LimitU	Observed	Expected
.	1.960	9.0	13.348
1.960	1.996	24.0	21.926
1.996	2.033	43.0	37.775
2.033	2.069	48.0	48.351
2.069	2.106	48.0	45.983
2.106	2.142	30.0	32.492
2.142	2.178	13.0	17.057
2.178	.	11.0	9.067
		226.000	226.000

Chi-square test statistic = 3.994580 df = 5 p-value = 0.550197

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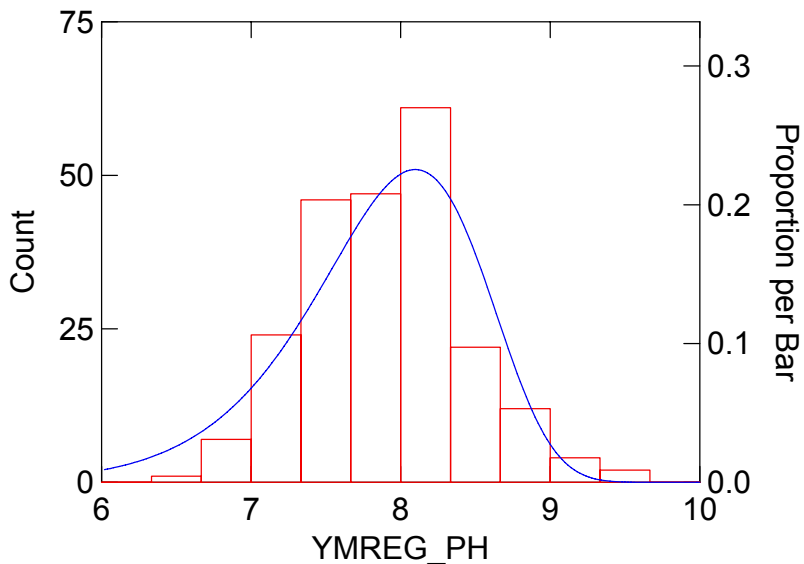
Kolmogorov-Smirnov test statistic = 0.058672 Lilliefors Probability (2-tail) = 0.056853
 Shapiro-Wilk test statistic for normality = 0.993254 p-value = 0.396730

Variable Name: YMREG_PH
 Distribution: Weibull
 Estimated: Scale (beta) = 8.135546 Shape (alpha) = 14.919605
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.600	1.0	9.755
6.600	6.890	5.0	8.414
6.890	7.180	8.0	14.288
7.180	7.470	30.0	22.717
7.470	7.760	55.0	32.933
7.760	8.050	45.0	41.692
8.050	8.340	42.0	43.092
8.340	8.630	22.0	32.843
8.630	.	18.0	20.266
		226.000	226.000

Chi-square test statistic = 33.254821 df = 6 p-value = 0.000009

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WARNING

One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.096363 p-value(2-tail) = 0.030075

Variable Name: TURNER_PH

Distribution: Normal

Estimated: Location or mean (μ) = 7.833261 Scale or SD (σ) = 0.445023

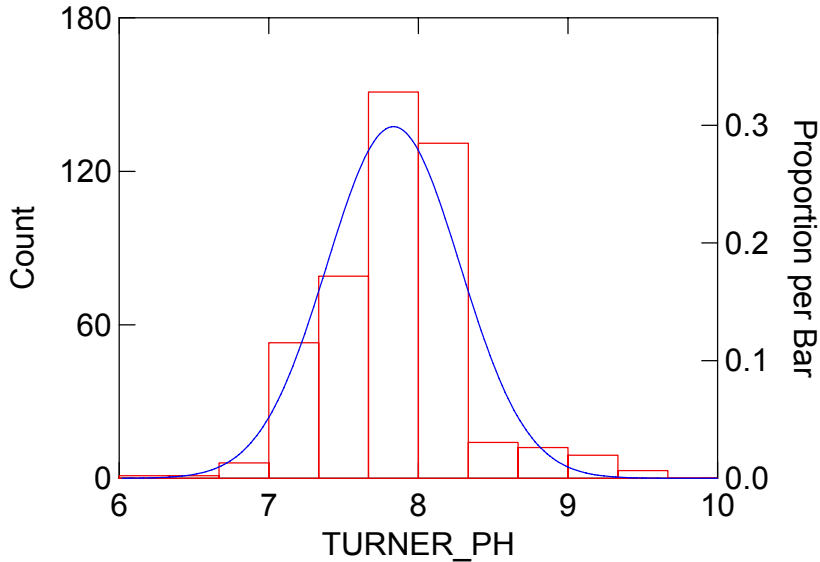
Estimation of parameter(s): Maximum likelihood method.

Test Results:

LimitL	LimitU	Observed	Expected
.	6.960	8.0	11.438
6.960	7.290	33.0	39.664
7.290	7.620	99.0	94.209
7.620	7.950	151.0	132.282
7.950	8.280	114.0	109.854
8.280	8.610	31.0	53.942
8.610	.	24.0	18.611
		460.000	460.000

Chi-square test statistic = 16.519708 df = 4 p-value = 0.002395

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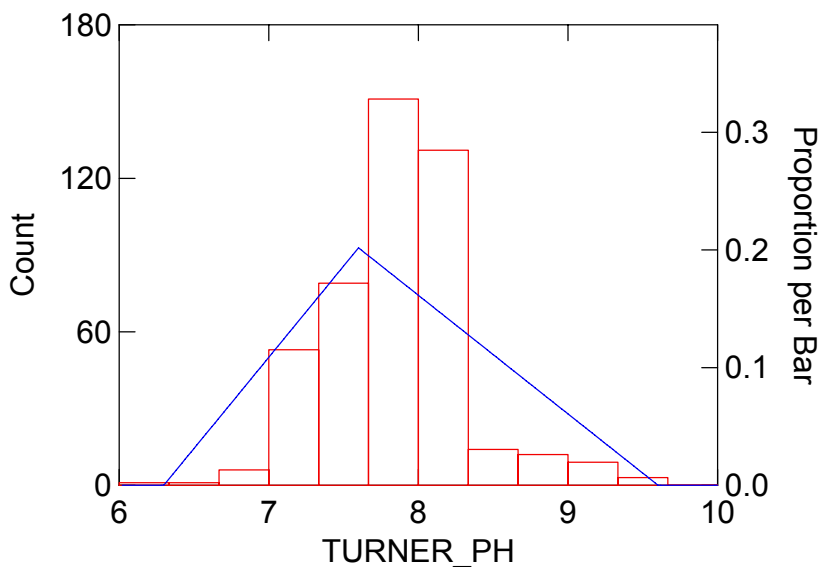
Kolmogorov-Smirnov test statistic = 0.096198 Lilliefors Probability (2-tail) = 0.000000
 Shapiro-Wilk test statistic for normality = 0.965539 p-value = 0.000000

Variable Name: TURNER_PH
 Distribution: Triangular
 Estimated: Low (a)=6.297826 High (b) = 9.602174 Mode (c) = 7.599783
 Estimation of parameter(s): Modified maximum likelihood and moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.630	2.0	11.798
6.630	6.960	6.0	35.086
6.960	7.290	33.0	58.374
7.290	7.620	99.0	81.590
7.620	7.950	151.0	83.380
7.950	8.280	114.0	68.238
8.280	8.610	31.0	53.096
8.610	8.940	12.0	37.955
8.940	9.270	8.0	22.813
9.270	.	4.0	7.671
		460.000	460.000

Chi-square test statistic = 170.838657 df = 6 p-value = 0.000000

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WARNING

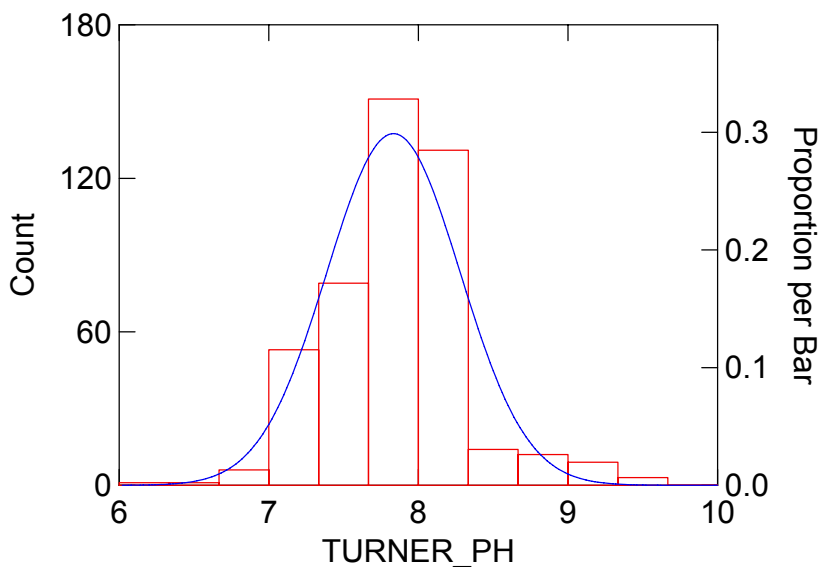
One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.187623 p-value(2-tail) = 0.000000

Variable Name: TURNER_PH
 Distribution: Gamma
 Estimated: Shape (alpha) = 309.827062 Scale (beta) = 0.025283
 Estimation of parameter(s): Method of moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.960	8.0	9.951
6.960	7.290	33.0	40.249
7.290	7.620	99.0	97.496
7.620	7.950	151.0	133.019
7.950	8.280	114.0	106.781
8.280	8.610	31.0	52.417
8.610	.	24.0	20.087
		460.000	460.000

Chi-square test statistic = 14.142875 df = 4 p-value = 0.006853

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WARNING

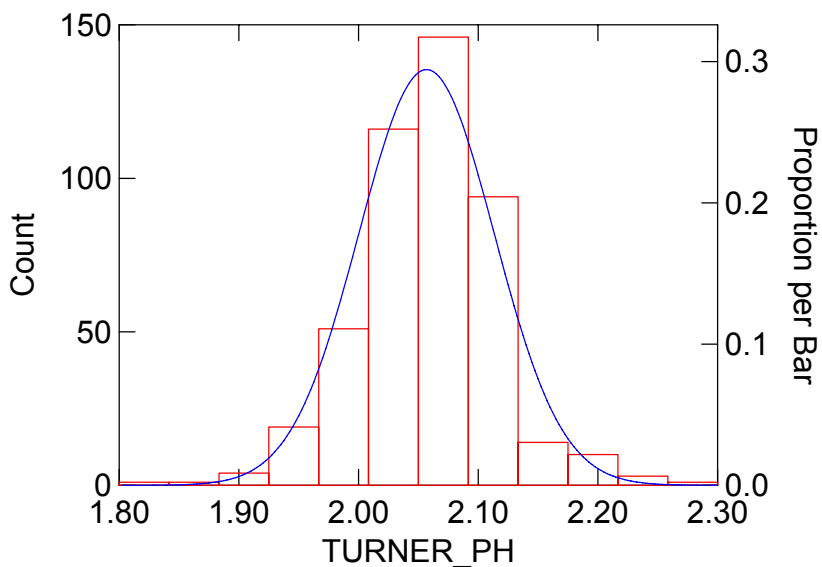
One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.098326 p-value(2-tail) = 0.000274

Variable Name: TURNER_PH
 Distribution: Lognormal
 Estimated: Location (mu) = 2.056780 Scale (sigma) = 0.056474
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:
 Log transformation is used on data.

LimitL	LimitU	Observed	Expected
.	1.967	25.0	25.656
1.967	2.009	51.0	65.855
2.009	2.051	116.0	120.246
2.051	2.093	186.0	129.080
2.093	2.135	54.0	81.470
2.135	2.178	14.0	30.214
2.178	.	14.0	7.479
		460.000	460.000

Chi-square test statistic = 52.265673 df = 4 p-value = 0.000000

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Kolmogorov-Smirnov test statistic = 0.099562 Lilliefors Probability (2-tail) = 0.000000
 Shapiro-Wilk test statistic for normality = 0.972169 p-value = 0.000000

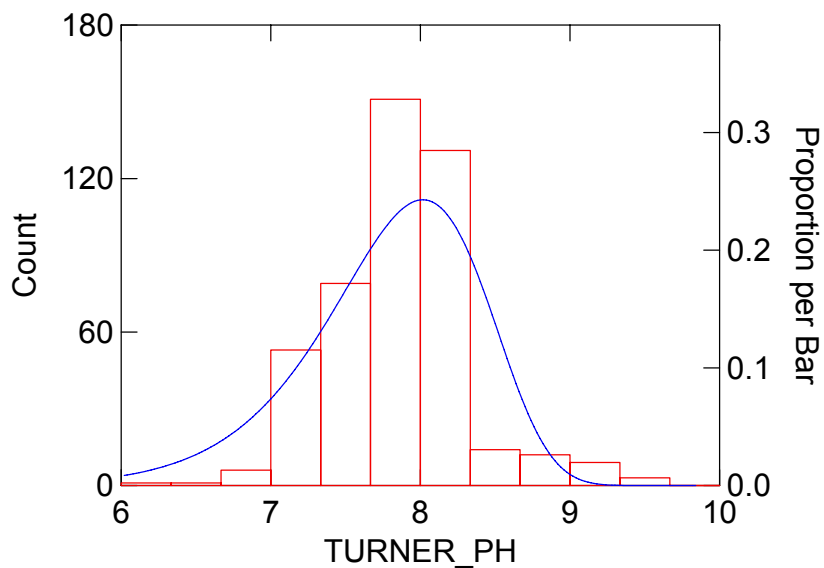
Variable Name: TURNER_PH
 Distribution: Weibull
 Estimated: Scale (beta) = 8.049142 Shape (alpha) = 15.909194
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.300	1.0	9.236
6.300	6.630	1.0	11.311
6.630	6.960	6.0	22.798
6.960	7.290	33.0	42.592
7.290	7.620	99.0	71.296
7.620	7.950	151.0	100.382
7.950	8.280	114.0	106.504
8.280	8.610	31.0	71.075
8.610	.	24.0	24.807
		460.000	460.000

Chi-square test statistic = 90.720580 df = 6 p-value = 0.000000

Of 200 cases, 8 were excluded by making graph range less than data range.

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One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.152818 p-value(2-tail) = 0.000000

Variable Name: SITE_PH

Distribution: Normal

Estimated: Location or mean (μ) = 7.867664 Scale or SD (σ) = 0.599530

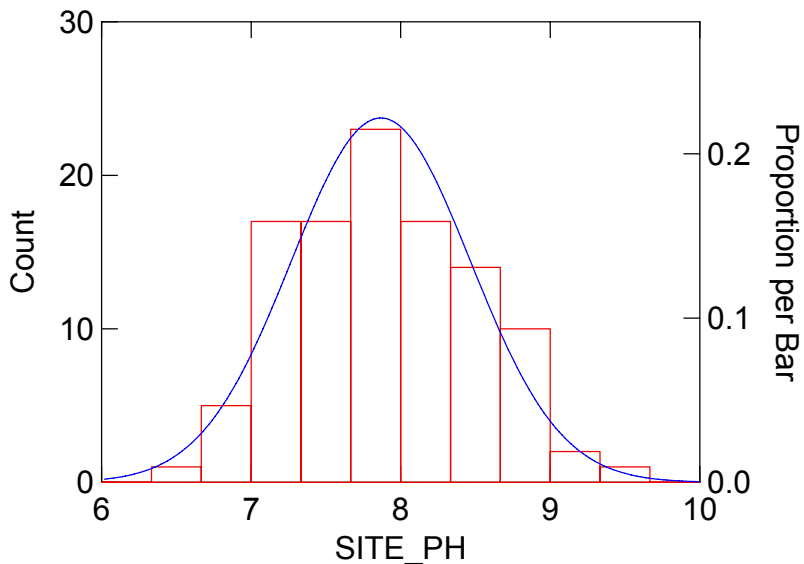
Estimation of parameter(s): Maximum likelihood method.

Test Results:

LimitL	LimitU	Observed	Expected
.	6.890	5.0	5.508
6.890	7.180	7.0	7.941
7.180	7.470	16.0	13.683
7.470	7.760	23.0	18.743
7.760	8.050	17.0	20.410
8.050	8.340	12.0	17.668
8.340	8.630	14.0	12.158
8.630	.	13.0	10.889
		107.000	107.000

Chi-square test statistic = 4.593505 df = 5 p-value = 0.467471

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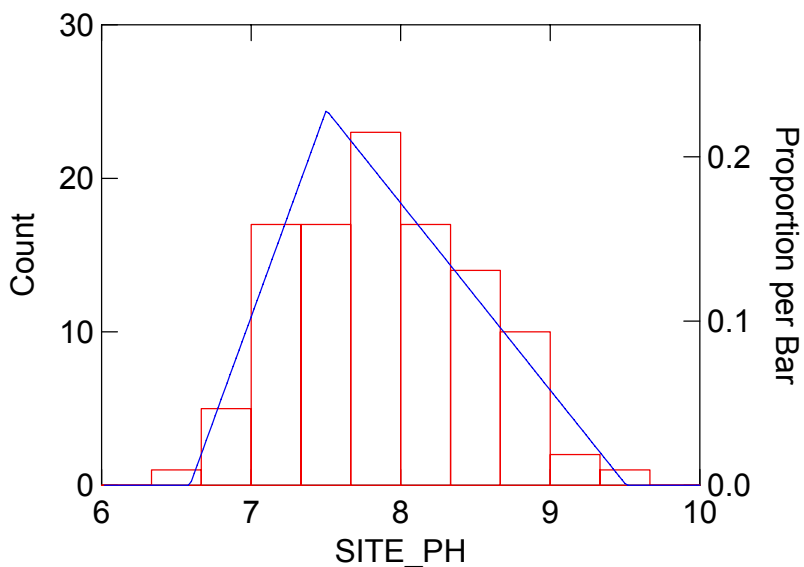
Kolmogorov-Smirnov test statistic = 0.068294 Lilliefors Probability (2-tail) = 0.233216
 Shapiro-Wilk test statistic for normality = 0.988236 p-value = 0.475610

Variable Name: SITE_PH
 Distribution: Triangular
 Estimated: Low (a)=6.590654 High (b) = 9.509346 Mode (c) = 7.502991
 Estimation of parameter(s): Modified maximum likelihood and moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	7.180	12.0	13.957
7.180	7.470	16.0	17.115
7.470	7.760	23.0	20.012
7.760	8.050	17.0	17.003
8.050	8.340	12.0	13.929
8.340	8.630	14.0	10.856
8.630	8.920	9.0	7.782
8.920	.	4.0	6.346
		107.000	107.000

Chi-square test statistic = 3.028810 df = 4 p-value = 0.553016

FITTED DISTRIBUTION



1-Jun-05 FPB

WARNING

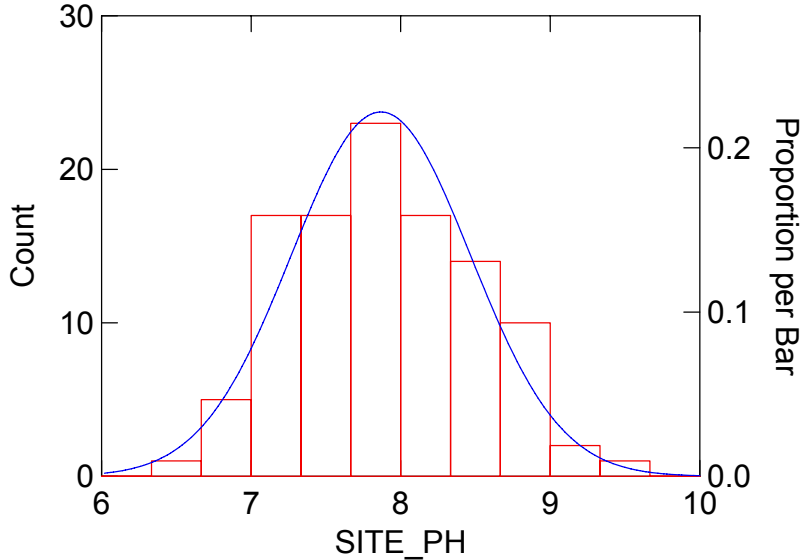
One or more parameters of distribution are estimated.
Significance of K-S test computed on this distribution is suspect.
Kolmogorov-Smirnov test statistic = 0.069040 p-value(2-tail) = 0.687554

Variable Name: SITE_PH
Distribution: Gamma
Estimated: Shape (alpha) = 172.214322 Scale (beta) = 0.045685
Estimation of parameter(s): Method of moments.
Test Results:

LimitL	LimitU	Observed	Expected
.	7.180	12.0	13.235
7.180	7.470	16.0	14.376
7.470	7.760	23.0	19.299
7.760	8.050	17.0	20.313
8.050	8.340	12.0	17.047
8.340	8.630	14.0	11.581
8.630	.	13.0	11.150
		107.000	107.000

Chi-square test statistic = 3.854737 df = 4 p-value = 0.426022

FITTED DISTRIBUTION



1-Jun-05 FPB

WARNING

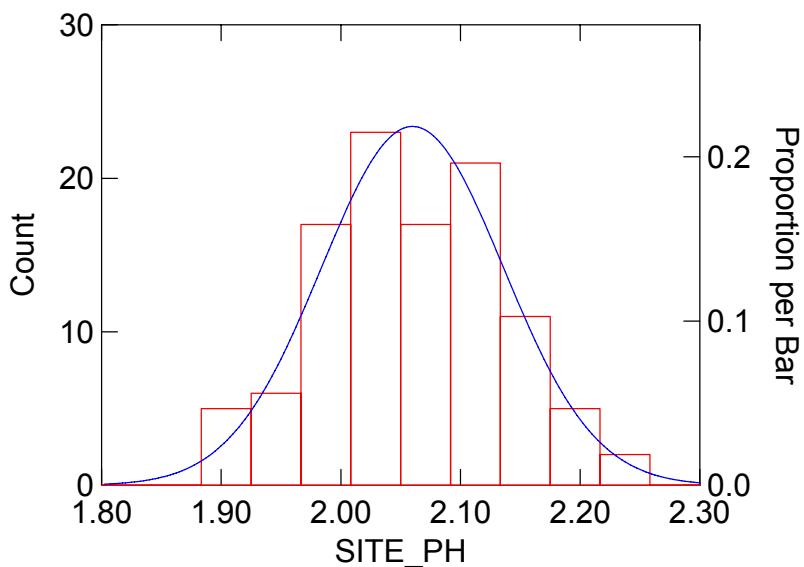
One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.062565 p-value(2-tail) = 0.796375

Variable Name: SITE_PH
 Distribution: Lognormal
 Estimated: Location (mu) = 2.059866 Scale (sigma) = 0.076086
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:
 Log transformation is used on data.

LimitL	LimitU	Observed	Expected
.	1.960	7.0	10.109
1.960	1.996	17.0	11.491
1.996	2.033	14.0	17.008
2.033	2.069	24.0	20.105
2.069	2.106	12.0	18.982
2.106	2.142	17.0	14.313
2.142	2.178	9.0	8.619
2.178	.	7.0	6.372
		107.000	107.000

Chi-square test statistic = 8.035412 df = 5 p-value = 0.154295

FITTED DISTRIBUTION



1-Jun-05 FPB

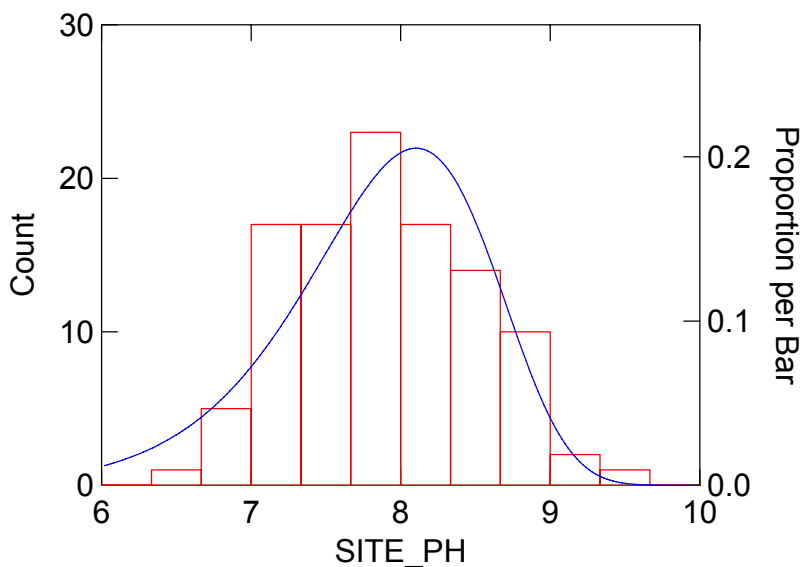
Kolmogorov-Smirnov test statistic = 0.064929 Lilliefors Probability (2-tail) = 0.296353
 Shapiro-Wilk test statistic for normality = 0.990611 p-value = 0.670332

Variable Name: SITE_PH
 Distribution: Weibull
 Estimated: Scale (beta) = 8.149405 Shape (alpha) = 13.602901
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.600	1.0	5.907
6.600	7.180	11.0	11.592
7.180	7.470	16.0	10.709
7.470	7.760	23.0	14.779
7.760	8.050	17.0	18.108
8.050	8.340	12.0	18.704
8.340	8.630	14.0	15.110
8.630	.	13.0	12.092
		107.000	107.000

Chi-square test statistic = 13.912671 df = 5 p-value = 0.016174

FITTED DISTRIBUTION



1-Jun-05 FPB

WARNING

One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.099762 p-value(2-tail) = 0.237321

	SITEMOD_PH	SITEMOD_CO2
N of cases	104	104
Minimum	6.700	-3.850
Maximum	9.200	-1.140
Range	2.500	2.710
Sum	819.040	-270.820
Median	7.800	-2.600
Mean	7.875	-2.604
95% CI Upper	7.985	-2.488
95% CI Lower	7.766	-2.720
Std. Error	0.055	0.058
Standard Dev	0.564	0.595
Variance	0.319	0.354
C.V.	0.072	-0.229
Skewness(G1)	0.167	0.239
SE Skewness	0.237	0.237
Kurtosis(G2)	-0.683	-0.303
SE Kurtosis	0.469	0.469
SW Statistic	0.983	0.988
SW P-Value	0.189	0.461

1-Jun-05 FPB

EM Algorithm	Iteration	Maximum Error	-2*log(likelihood)
	1	1.000	2557.516
	2	0.000	-391.637

No. of Cases	Missing value patterns (X=nonmissing; .=missing)
104	XX
692	..

Little MCAR test statistic: 0.000 df = 0 prob = .

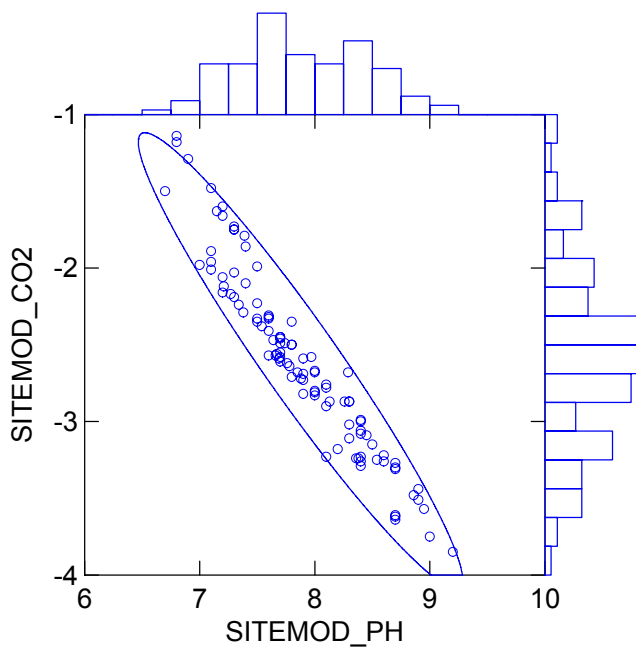
EM estimate of means

SITEMOD_PH	SITEMOD_CO2
7.875	-2.604

EM estimated correlation matrix

	SITEMOD_PH	SITEMOD_CO2
SITEMOD_PH	1.000	
SITEMOD_CO2	-0.959	1.000

Number of observations: 104



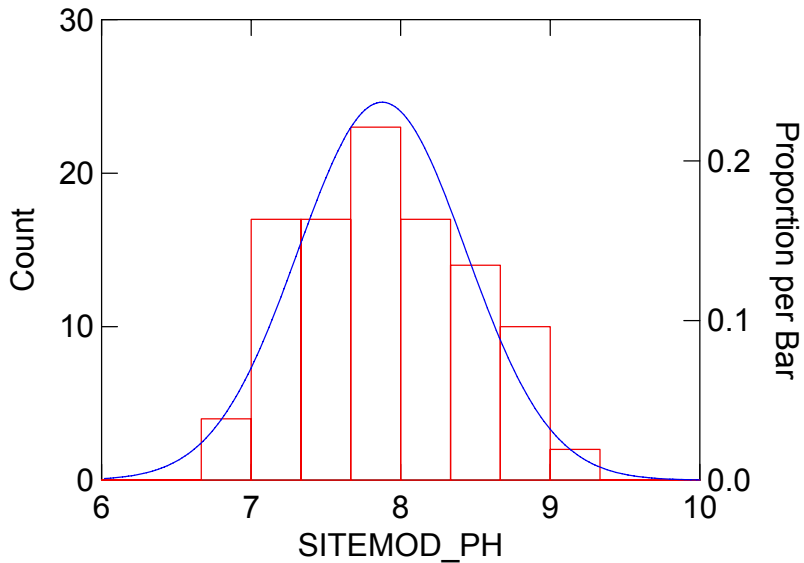
1-Jun-05 FPB

Variable Name: SITEMOD_PH
 Distribution: Normal
 Estimated: Location or mean (μ) = 7.875385 Scale or SD (σ) = 0.561750
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.950	4.0	5.174
6.950	7.200	10.0	6.748
7.200	7.450	12.0	11.422
7.450	7.700	21.0	15.911
7.700	7.950	13.0	18.241
7.950	8.200	12.0	17.211
8.200	8.450	16.0	13.364
8.450	8.700	10.0	8.540
8.700	.	6.0	7.390
		104.000	104.000

Chi-square test statistic = 7.605369 df = 6 p-value = 0.268463

FITTED DISTRIBUTION



1-Jun-05 FPB

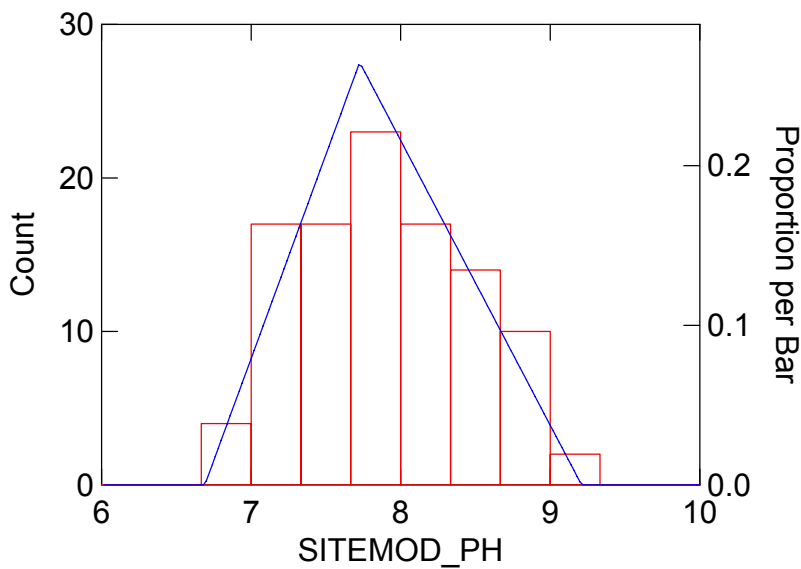
Kolmogorov-Smirnov test statistic = 0.074483 Lilliefors Probability (2-tail) = 0.156148
 Shapiro-Wilk test statistic for normality = 0.982587 p-value = 0.189456

Variable Name: SITEMOD_PH
 Distribution: Triangular
 Estimated: Low (a)=6.690385 High (b) = 9.209615 Mode (c) = 7.726154
 Estimation of parameter(s): Modified maximum likelihood and moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	7.200	14.0	10.351
7.200	7.450	12.0	12.647
7.450	7.700	21.0	17.629
7.700	7.950	13.0	19.220
7.950	8.200	12.0	15.787
8.200	8.450	16.0	12.309
8.450	8.700	10.0	8.830
8.700	.	6.0	7.227
		104.000	104.000

Chi-square test statistic = 6.355553 df = 4 p-value = 0.174122

FITTED DISTRIBUTION



1-Jun-05 FPB

WARNING

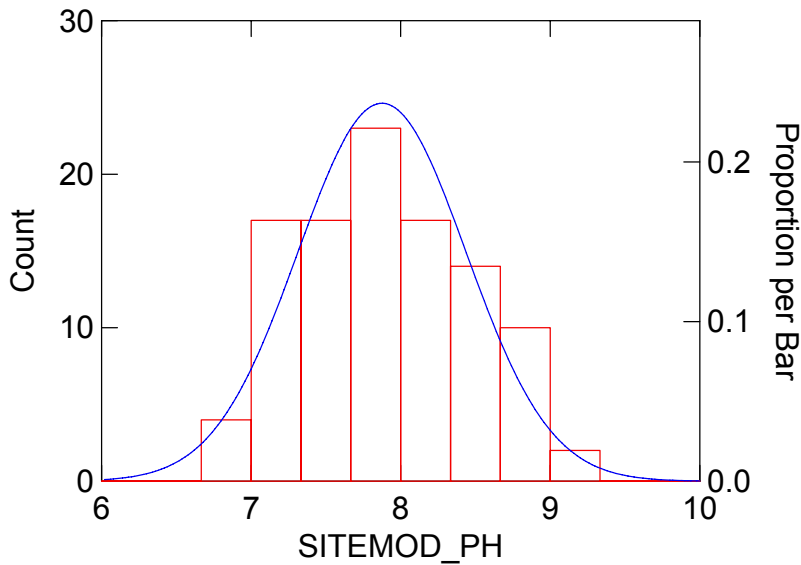
One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.071785 p-value(2-tail) = 0.657394

Variable Name: SITEMOD_PH
 Distribution: Gamma
 Estimated: Shape (alpha) = 196.542754 Scale (beta) = 0.040070
 Estimation of parameter(s): Method of moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	7.200	14.0	11.675
7.200	7.450	12.0	11.972
7.450	7.700	21.0	16.457
7.700	7.950	13.0	18.351
7.950	8.200	12.0	16.811
8.200	8.450	16.0	12.801
8.450	8.700	10.0	8.189
8.700	.	6.0	7.745
		104.000	104.000

Chi-square test statistic = 6.247802 df = 5 p-value = 0.282848

FITTED DISTRIBUTION



WARNING

One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.071229 p-value(2-tail) = 0.666961

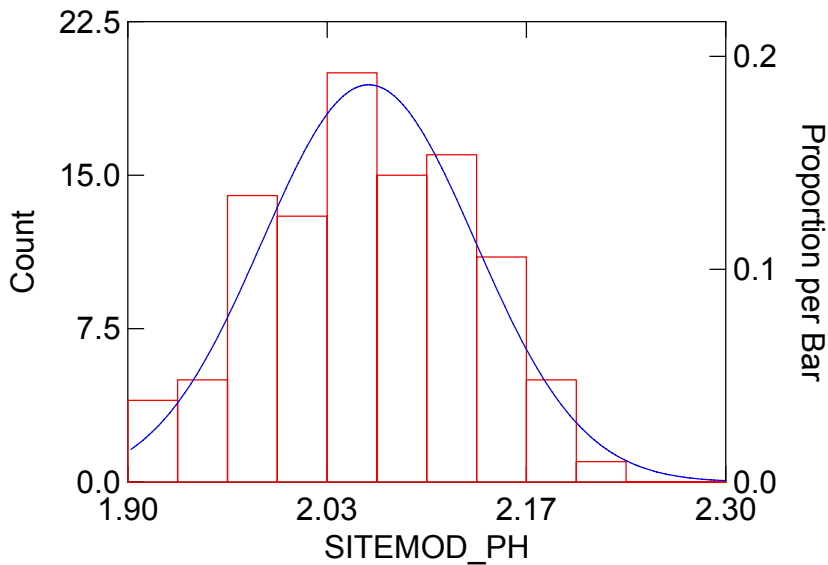
1-Jun-05 FPB

Variable Name: SITEMOD_PH
 Distribution: Lognormal
 Estimated: Location (mu) = 2.061203 Scale (sigma) = 0.071242
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:
 Log transformation is used on data.

LimitL	LimitU	Observed	Expected
.	1.966	9.0	9.323
1.966	1.997	13.0	9.878
1.997	2.029	14.0	14.636
2.029	2.061	19.0	17.844
2.061	2.092	15.0	17.905
2.092	2.124	9.0	14.784
2.124	2.156	13.0	10.046
2.156	.	12.0	9.584
		104.000	104.000

Chi-square test statistic = 5.311665 df = 5 p-value = 0.379039

FITTED DISTRIBUTION



Kolmogorov-Smirnov test statistic = 0.073199 Lilliefors Probability (2-tail) = 0.172957
 Shapiro-Wilk test statistic for normality = 0.984871 p-value = 0.285236

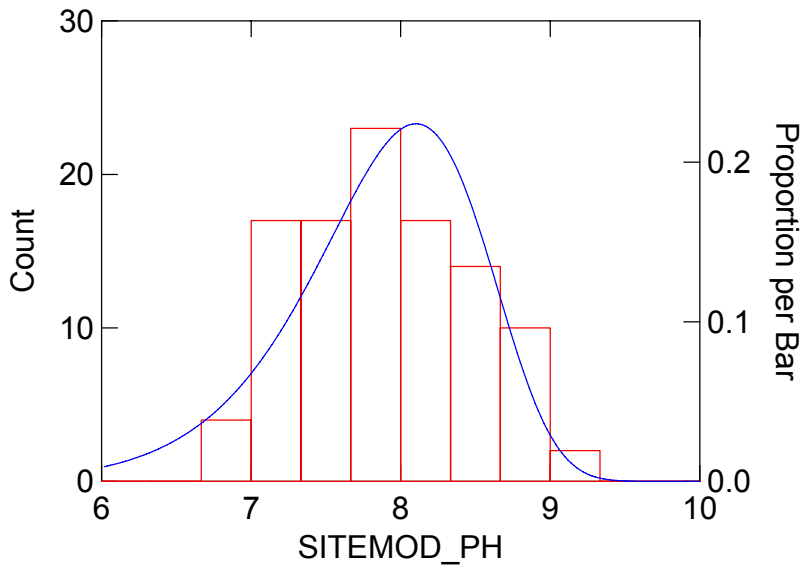
1-Jun-05 FPB

Variable Name: SITEMOD_PH
 Distribution: Weibull
 Estimated: Scale (beta) = 8.140596 Shape (alpha) = 14.835721
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:

LimitL	LimitU	Observed	Expected
.	6.700	1.0	5.626
6.700	7.200	13.0	9.908
7.200	7.450	12.0	8.950
7.450	7.700	21.0	12.404
7.700	7.950	13.0	15.656
7.950	8.200	12.0	17.316
8.200	8.450	16.0	15.872
8.450	8.700	10.0	11.141
8.700	.	6.0	7.128
		104.000	104.000

Chi-square test statistic = 14.145167 df = 6 p-value = 0.028056

FITTED DISTRIBUTION



WARNING
 One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.107585 p-value(2-tail) = 0.179950

1-Jun-05 FPB

Variable Name: SITEMOD_CO2

Distribution: Normal

Estimated: Location or mean (μ) = -2.604038 Scale or SD (σ) = 0.592341

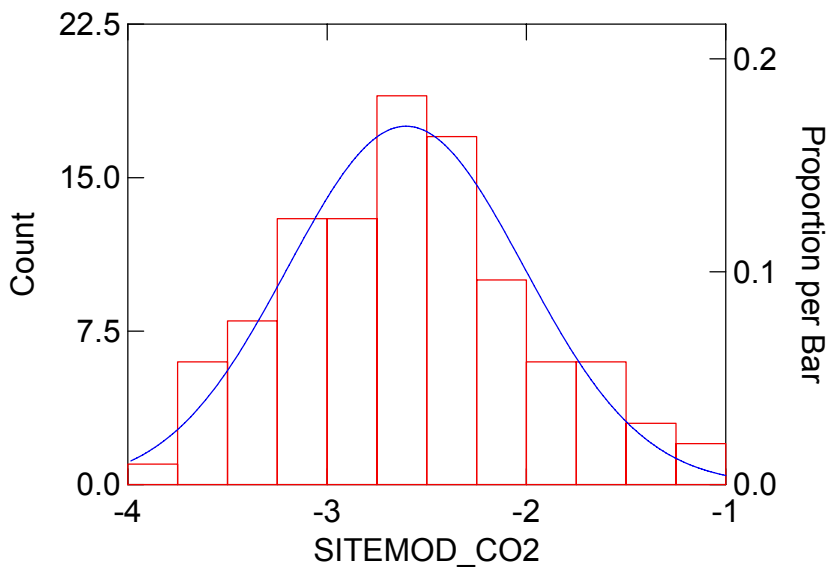
Estimation of parameter(s): Maximum likelihood method.

Test Results:

LimitL	LimitU	Observed	Expected
.	-3.579	5.0	5.188
-3.579	-3.308	5.0	7.014
-3.308	-3.037	17.0	11.968
-3.037	-2.766	13.0	16.625
-2.766	-2.495	22.0	18.799
-2.495	-2.224	17.0	17.306
-2.224	-1.953	11.0	12.970
-1.953	-1.682	6.0	7.912
-1.682	.	8.0	6.217
		104.000	104.000

Chi-square test statistic = 5.313632 df = 6 p-value = 0.504262

FITTED DISTRIBUTION



Kolmogorov-Smirnov test statistic = 0.052724 Lilliefors Probability (2-tail) = 0.632850
 Shapiro-Wilk test statistic for normality = 0.987746 p-value = 0.460637

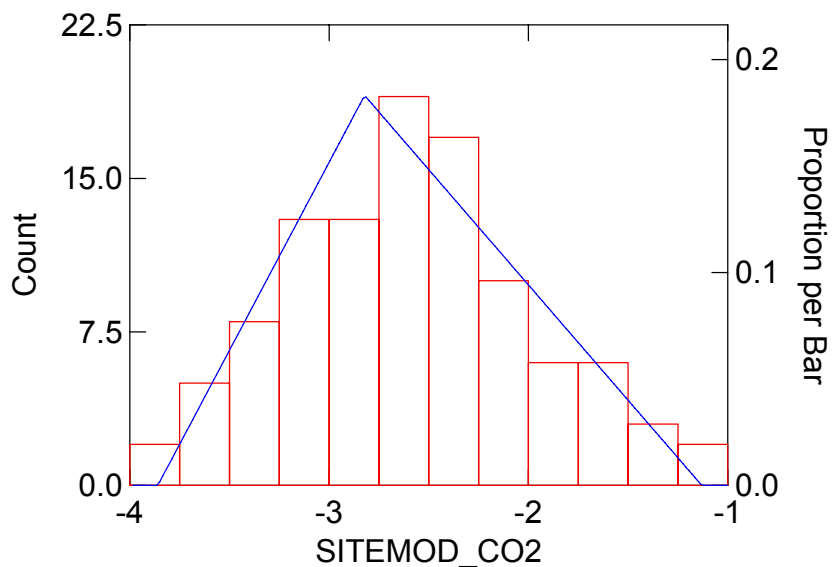
1-Jun-05 FPB

Variable Name: SITEMOD_CO2
 Distribution: Triangular
 Estimated: Low (a)=-3.859615 High (b) = -1.130385 Mode (c) = -2.822115
 Estimation of parameter(s): Modified maximum likelihood and moments.
 Test Results:

LimitL	LimitU	Observed	Expected
.	-3.308	10.0	11.176
-3.308	-3.037	17.0	13.678
-3.037	-2.766	13.0	18.887
-2.766	-2.495	22.0	18.314
-2.495	-2.224	17.0	15.006
-2.224	-1.953	11.0	11.697
-1.953	-1.682	6.0	8.389
-1.682	.	8.0	6.854
		104.000	104.000

Chi-square test statistic = 4.685301 df = 4 p-value = 0.321137

FITTED DISTRIBUTION



WARNING

One or more parameters of distribution are estimated.
 Significance of K-S test computed on this distribution is suspect.
 Kolmogorov-Smirnov test statistic = 0.057443 p-value(2-tail) = 0.882507

1-Jun-05 FPB

Variable Name: SITEMOD_CO2

ERROR

This dataset is not appropriate for fitting a Gamma distribution.

Variable Name: SITEMOD_CO2

ERROR

This dataset is not appropriate for fitting a Lognormal distribution.

Variable Name: SITEMOD_CO2

ERROR

This dataset is not appropriate for fitting a Weibull distribution.

Variable Name: SITEMOD_CO2

Distribution: Triangular

Specified: Low (a)=-4.000000 High (b) = -1.000000 Mode (c) = -2.600000

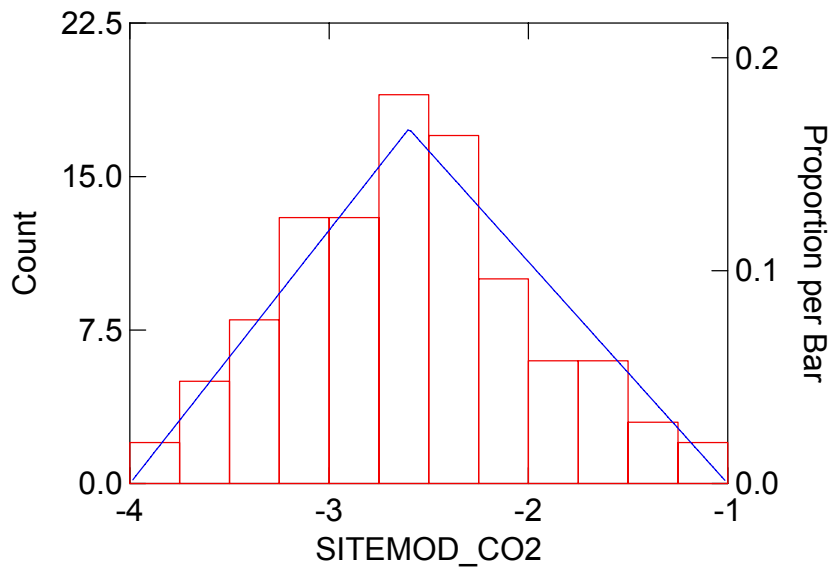
Test Results:

LimitL	LimitU	Observed	Expected
.	-3.308	10.0	11.858
-3.308	-3.037	17.0	11.106
-3.037	-2.766	13.0	14.743
-2.766	-2.495	22.0	17.868
-2.495	-2.224	17.0	15.965
-2.224	-1.953	11.0	12.783
-1.953	-1.682	6.0	9.600
-1.682	.	8.0	10.078
		104.000	104.000

Chi-square test statistic = 6.674856 df = 7 p-value = 0.463500

Of 200 cases, 1 were excluded by making graph range less than data range.

FITTED DISTRIBUTION



Kolmogorov-Smirnov test statistic = 0.091867 p-value(2-tail) = 0.343883

1-Jun-05 FPB

07-Jun-07 FPB

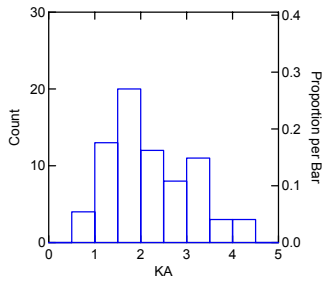
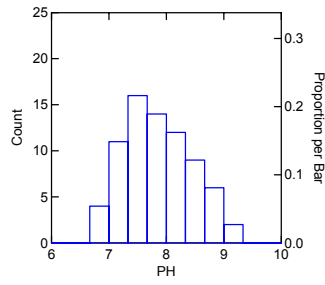
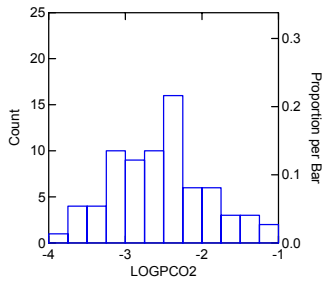
74 cases and 18 variables processed and saved.

SYSTAT Rectangular file D:\Systat_data\YM_Wells_KA.syd,
 created Thu Jun 07, 2007 at 10:56:57, contains variables:

NUMBER	WELL\$	X_METERS	Y_METERS	LOGPCO2	PH
KA	TEMP_C	CA	MG	NA	K
CL	SO4	HCO3	CO3	F	SIO2

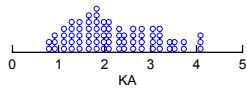
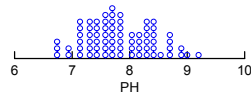
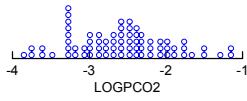
	LOGPCO2	PH	KA
N of cases	74	74	74
Minimum	-3.850	6.700	0.747
Maximum	-1.140	9.200	4.087
Range	2.710	2.500	3.340
Sum	-189.870	579.610	162.772
Median	-2.555	7.720	1.989
Mean	-2.566	7.833	2.200
95% CI Upper	-2.423	7.965	2.397
95% CI Lower	-2.708	7.700	2.002
Std. Error	0.072	0.066	0.099
Standard Dev	0.615	0.571	0.852
Variance	0.378	0.326	0.726
C.V.	-0.240	0.073	0.387
Skewness(G1)	0.171	0.243	0.429
SE Skewness	0.279	0.279	0.279
Kurtosis(G2)	-0.275	-0.499	-0.618
SE Kurtosis	0.552	0.552	0.552
SW Statistic	0.989	0.983	0.965
SW P-Value	0.759	0.416	0.038

07-Jun-07 FPB



07-Jun-07

FPB

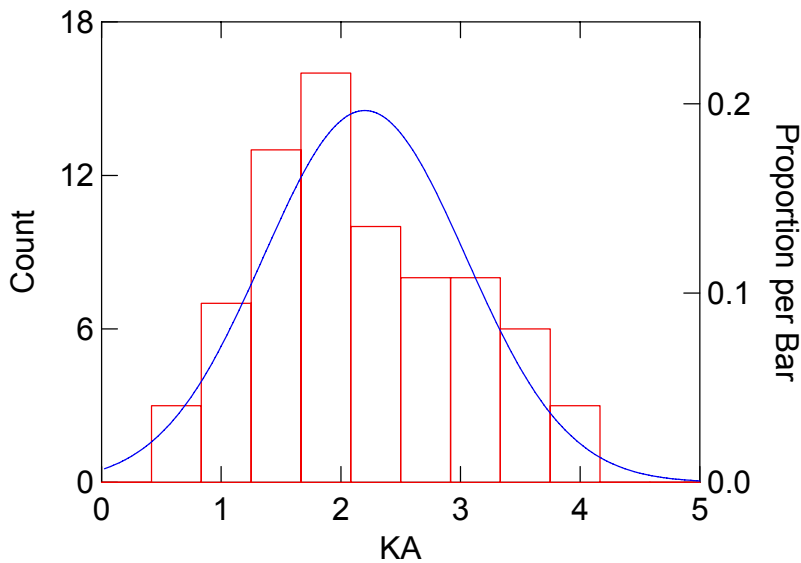


Variable Name: KA
 Distribution: Normal
 Estimated: Location or mean (μ) = 2.199624 Scale or SD (σ) = 0.846290
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:

LimitL	LimitU	Observed	Expected
.	1.081	5.0	6.891
1.081	1.415	10.0	6.201
1.415	1.749	9.0	8.899
1.749	2.083	15.0	10.950
2.083	2.417	7.0	11.555
2.417	2.751	7.0	10.455
2.751	3.085	7.0	8.112
3.085	3.419	7.0	5.398
3.419	.	7.0	5.539
		74.000	74.000

Chi-square test statistic = 8.295505 df = 6 p-value = 0.217243

FITTED DISTRIBUTION



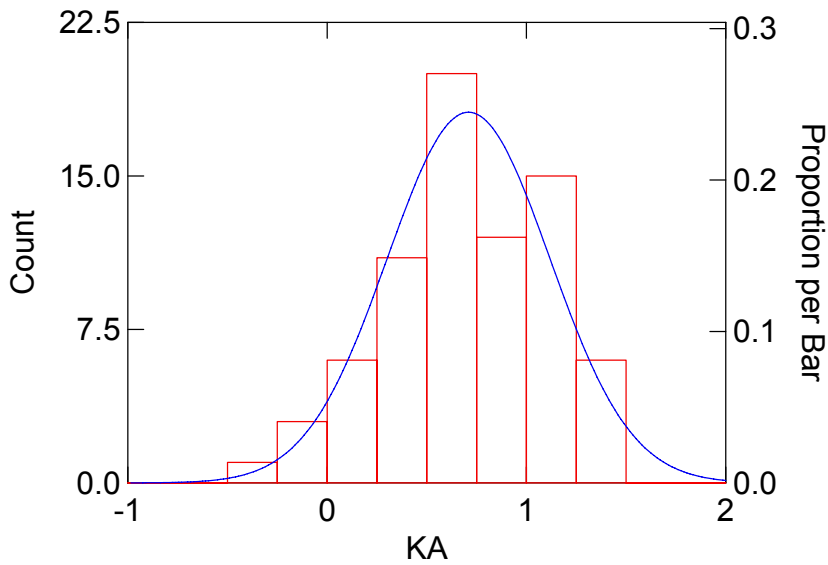
Kolmogorov-Smirnov test statistic = 0.105127 Lilliefors Probability (2-tail) = 0.041712
 Shapiro-Wilk test statistic for normality = 0.964919 p-value = 0.037711

Variable Name: KA
 Distribution: Lognormal
 Estimated: Location (mu) = 0.709554 Scale (sigma) = 0.407521
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:
 Log transformation is used on data.

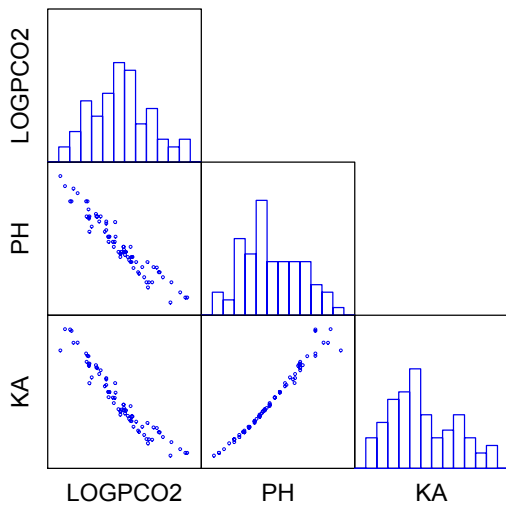
LimitL	LimitU	Observed	Expected
.	0.218	10.0	8.432
0.218	0.388	6.0	7.486
0.388	0.558	8.0	10.353
0.558	0.728	15.0	12.063
0.728	0.898	10.0	11.841
0.898	1.068	8.0	9.792
1.068	1.238	11.0	6.822
1.238	.	6.0	7.211
		74.000	74.000

Chi-square test statistic = 5.212735 df = 5 p-value = 0.390473

FITTED DISTRIBUTION



Kolmogorov-Smirnov test statistic = 0.060037 Lilliefors Probability (2-tail) = 0.704131
 Shapiro-Wilk test statistic for normality = 0.976343 p-value = 0.179198



07-Jun-07

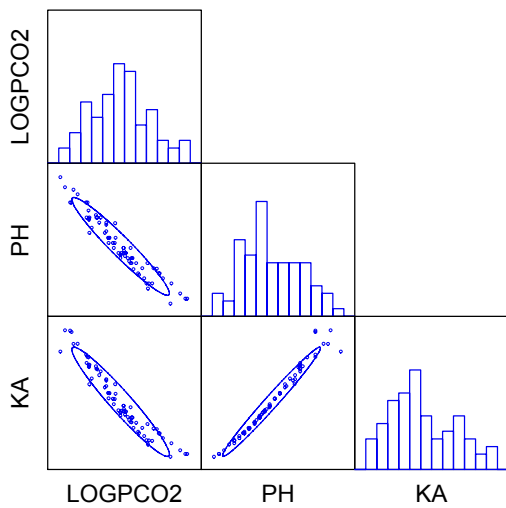
FPB

Means

	LOGPCO2	PH	KA
	-2.566	7.833	2.200

Pearson correlation matrix

	LOGPCO2	PH	KA
LOGPCO2	1.000		
PH	-0.959	1.000	
KA	-0.958	0.985	1.000



Bartlett Chi-square statistic: 434.381 df=3 Prob= 0.000

Matrix of Bonferroni Probabilities

	LOGPCO2	PH	KA
LOGPCO2	0.000		
PH	0.000	0.000	
KA	0.000	0.000	0.000

Number of observations: 74

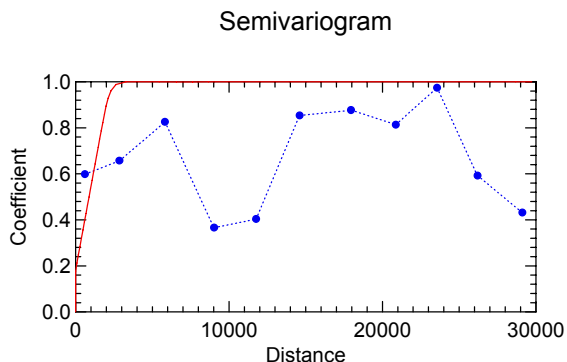
07-Jun-07 FPB

Structural Model

Nugget (c0): 0.000000
 First rotation angle (azimuth, or degrees clockwise from North): 0.000000
 Second rotation angle (dip, or degrees down from azimuthal): 0.000000
 First anisotropy index (anis1=ahmin/ahmax): 1.000000
 Sill (c): 1.000000
 Range (a): 1.000000

Semivariogram

Direction: 0.000000
 Number of lags: 10
 Lag distance: 2972.899902
 Lag tolerance: 1486.449951
 Angular tolerance: 90.000000
 Maximum horizontal bandwidth: 2972.899902



Structural Model

Nugget (c0): 0.000000
 First rotation angle (azimuth, or degrees clockwise from North): 0.000000
 Second rotation angle (dip, or degrees down from azimuthal): 0.000000
 First anisotropy index (anis1=ahmin/ahmax): 1.000000
 Sill (c): 1.000000
 Range (a): 1.000000

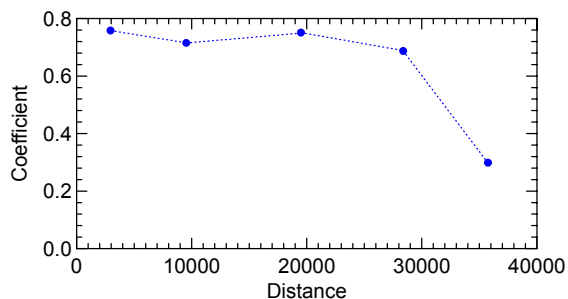
Semivariogram

Direction: 0.000000
 Number of lags: 25
 Lag distance: 10000.000000
 Lag tolerance: 5000.000000

Angular tolerance: 90.000000
Maximum horizontal bandwidth: 10000.000000

Of 5 cases, 4 were excluded by making graph range less than data range.

Semivariogram



07-Jun-07

FPB

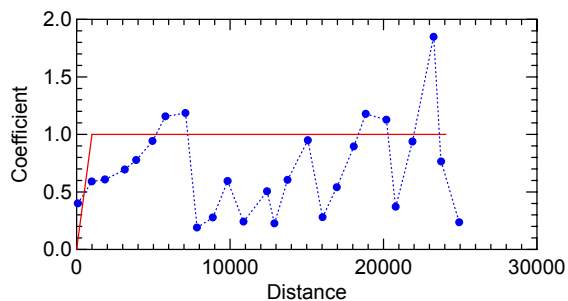
Structural Model

Nugget (c0): 0.000000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 1.000000
Range (a): 1.000000

Semivariogram

Direction: 0.000000
Number of lags: 25
Lag distance: 1000.000000
Lag tolerance: 500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 1000.000000

Semivariogram



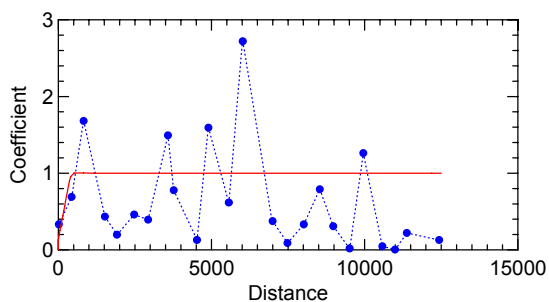
Structural Model

Nugget (c0): 0.000000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000

Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 1.000000
Range (a): 1.000000

Semivariogram
Direction: 0.000000
Number of lags: 25
Lag distance: 500.000000
Lag tolerance: 250.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 500.000000

Semivariogram



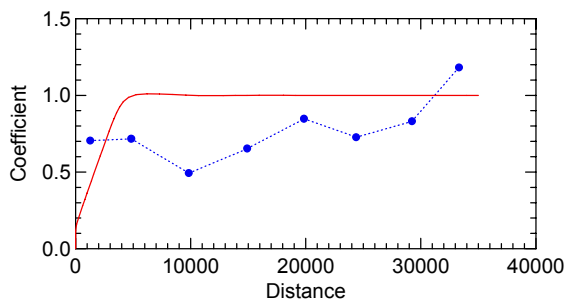
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Structural Model
Nugget (c0): 0.000000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 1.000000
Range (a): 1.000000

Semivariogram
Direction: 0.000000
Number of lags: 25
Lag distance: 5000.000000
Lag tolerance: 2500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 5000.000000

Semivariogram



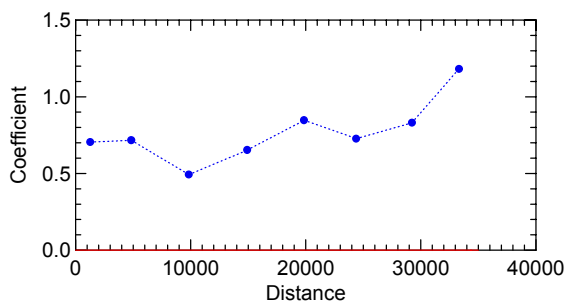
Structural Model

Nugget (c0): 0.000000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 1.000000
Range (a): 1.000000

Semivariogram

Direction: 0.000000
Number of lags: 25
Lag distance: 5000.000000
Lag tolerance: 2500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 5000.000000

Semivariogram



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Structural Model

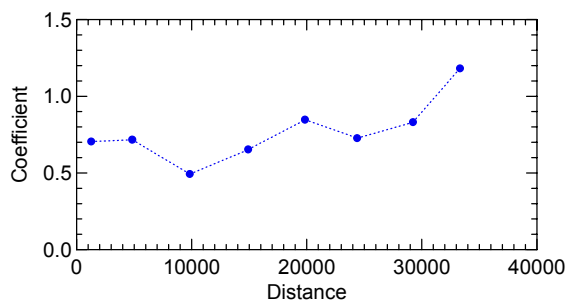
Nugget (c0): 0.000000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 1.000000
Range (a): 1.000000

Semivariogram

Direction: 0.000000
Number of lags: 25
Lag distance: 5000.000000
Lag tolerance: 2500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 5000.000000

Of 8 cases, 7 were excluded by making graph range less than data range.

Semivariogram



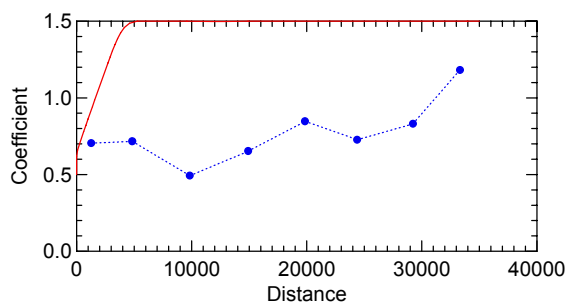
Structural Model

Nugget (c0): 0.500000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 1.000000
Range (a): 1.000000

Semivariogram

Direction: 0.000000
Number of lags: 25
Lag distance: 5000.000000
Lag tolerance: 2500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 5000.000000

Semivariogram



Structural Model

Nugget (c0): 0.500000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 5000.000000
Range (a): 1.000000

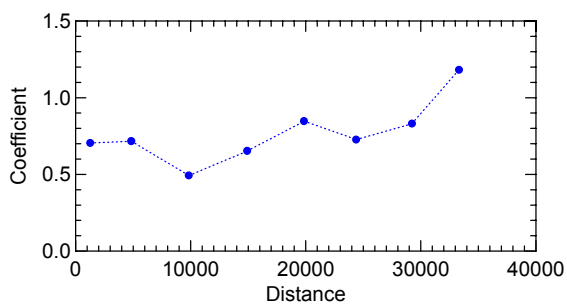
Semivariogram

Direction: 0.000000

Number of lags: 25
Lag distance: 5000.000000
Lag tolerance: 2500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 5000.000000

Of 8 cases, 7 were excluded by making graph range less than data range.

Semivariogram



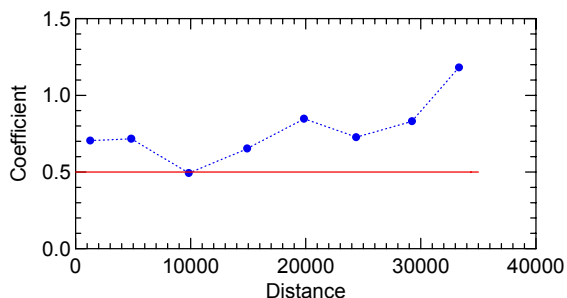
Structural Model

Nugget (c0): 0.500000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 0.000000
Range (a): 1.000000

Semivariogram

Direction: 0.000000
Number of lags: 25
Lag distance: 5000.000000
Lag tolerance: 2500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 5000.000000

Semivariogram



Structural Model

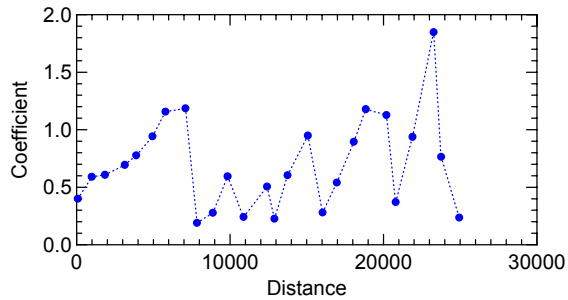
Nugget (c0): 0.500000
First rotation angle (azimuth, or degrees clockwise from North): 0.000000
Second rotation angle (dip, or degrees down from azimuthal): 0.000000
First anisotropy index (anis1=ahmin/ahmax): 1.000000
Sill (c): 500.000000
Range (a): 1.000000

Semivariogram
Direction: 0.000000
Number of lags: 25
Lag distance: 1000.000000
Lag tolerance: 500.000000
Angular tolerance: 90.000000
Maximum horizontal bandwidth: 1000.000000

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Of 26 cases, 25 were excluded by making graph range less than data range.

Semivariogram



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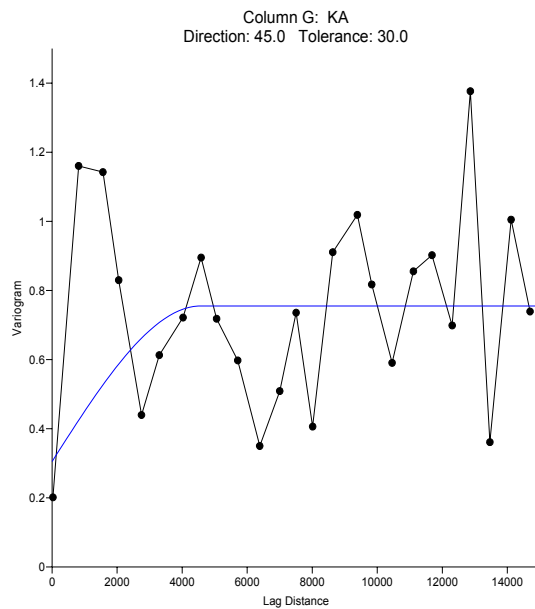
FPB

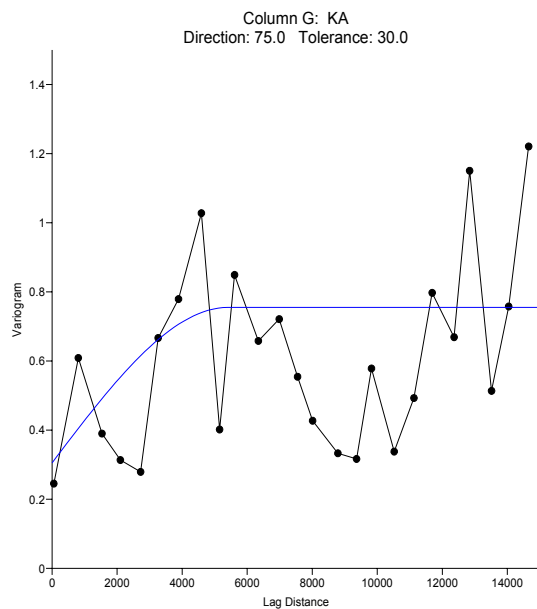
Alex,

The data for the KA model is provided below and in the associated files. Variogram results are not too good, even after I have selected the best data set.

Spherical Model, Scale= 0.45 , Length= 5540, Anisotropy= Ratio:2, Angle: 68.2
Nugget= 0.3053

The data could be fit using a linear model as well. Neither model is particularly good. Is it possible that there is no distinct spatial correlation/distribution? Could we simply model the system using the mean and variance without a spatially constrained effect for the chemistry?





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Here are some basis statistics for the chemistry data

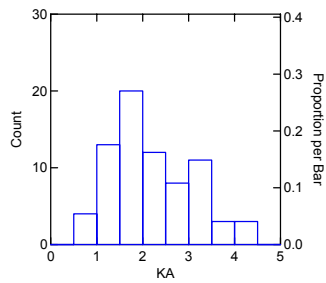
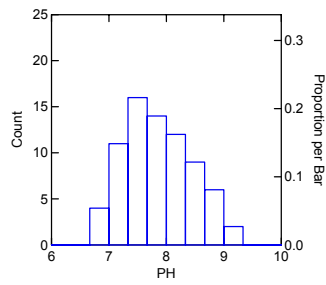
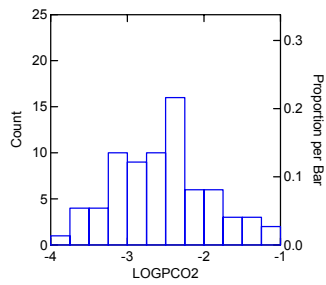
74 cases and 18 variables processed and saved.

SYSTAT Rectangular file D:\Systat_data\YM_Wells_KA.syd,
created Thu Jun 07, 2007 at 10:56:57, contains variables:

NUMBER	WELL\$	X_METERS	Y_METERS	LOGPCO2	PH
KA	TEMP_C	CA	MG	NA	K
CL	SO4	HCO3	CO3	F	SIO2

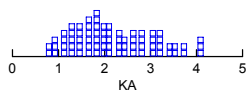
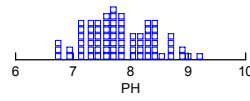
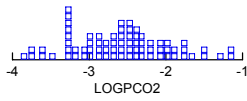
	LOGPCO2	PH	KA
N of cases	74	74	74
Minimum	-3.850	6.700	0.747
Maximum	-1.140	9.200	4.087
Range	2.710	2.500	3.340
Sum	-189.870	579.610	162.772
Median	-2.555	7.720	1.989
Mean	-2.566	7.833	2.200
95% CI Upper	-2.423	7.965	2.397
95% CI Lower	-2.708	7.700	2.002
Std. Error	0.072	0.066	0.099
Standard Dev	0.615	0.571	0.852
Variance	0.378	0.326	0.726
C.V.	-0.240	0.073	0.387
Skewness(G1)	0.171	0.243	0.429
SE Skewness	0.279	0.279	0.279
Kurtosis(G2)	-0.275	-0.499	-0.618
SE Kurtosis	0.552	0.552	0.552
SW Statistic	0.989	0.983	0.965
SW P-Value	0.759	0.416	0.038

**Note: logPCO₂ on the top left, pH on the top right, K_A on the bottom
pH and CO₂ are log-normally distributed, K_A appears normally distributed.**



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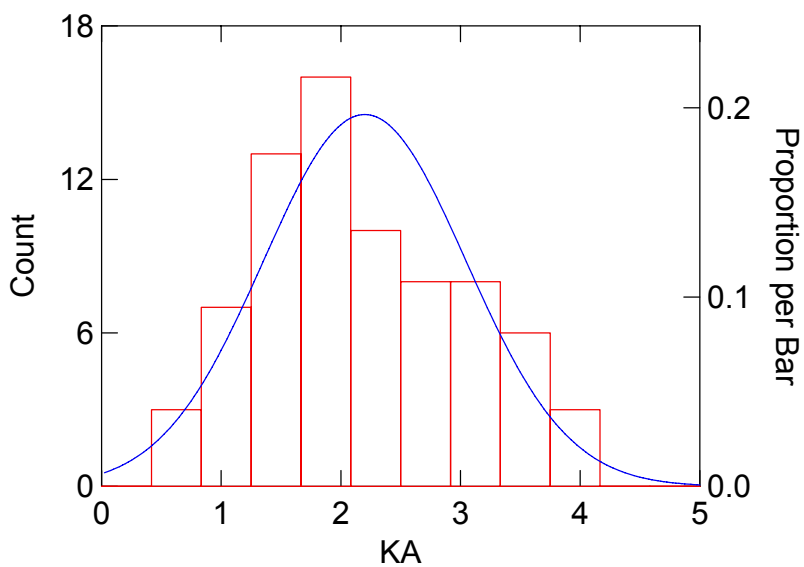
Variable Name: KA
Distribution: Normal
Estimated: Location or mean (μ) = 2.199624 Scale or SD (σ) = 0.846290
Estimation of parameter(s): Maximum likelihood method.
Test Results:

LimitL	LimitU	Observed	Expected
.	1.081	5.0	6.891
1.081	1.415	10.0	6.201
1.415	1.749	9.0	8.899
1.749	2.083	15.0	10.950
2.083	2.417	7.0	11.555
2.417	2.751	7.0	10.455
2.751	3.085	7.0	8.112
3.085	3.419	7.0	5.398
3.419	.	7.0	5.539
		74.000	74.000

Chi-square test statistic = 8.295505 df = 6 p-value = 0.217243

Looks like a normal or log-normal distribution will work for the K_A data

FITTED DISTRIBUTION



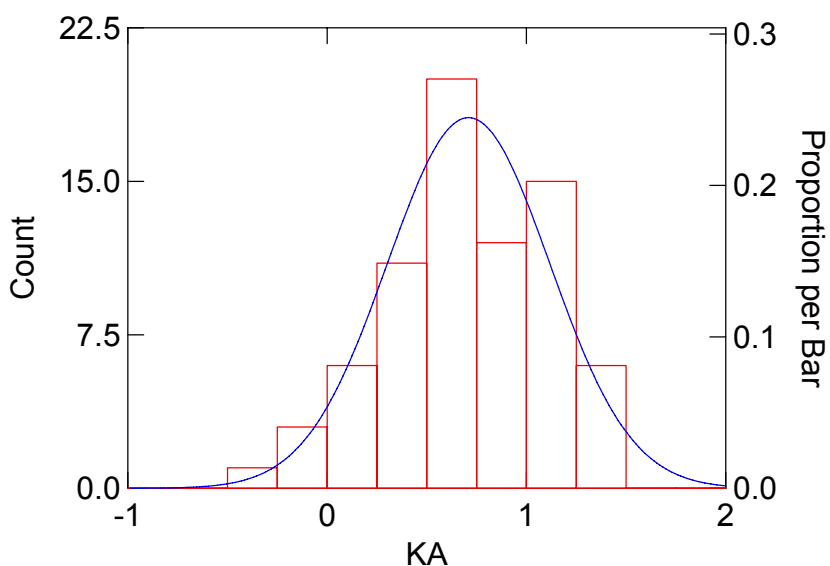
Kolmogorov-Smirnov test statistic = 0.105127 Lilliefors Probability (2-tail) = 0.041712
 Shapiro-Wilk test statistic for normality = 0.964919 p-value = 0.037711

Variable Name: KA
 Distribution: Lognormal
 Estimated: Location (mu) = 0.709554 Scale (sigma) = 0.407521
 Estimation of parameter(s): Maximum likelihood method.
 Test Results:
 Log transformation is used on data.

LimitL	LimitU	Observed	Expected
.	0.218	10.0	8.432
0.218	0.388	6.0	7.486
0.388	0.558	8.0	10.353
0.558	0.728	15.0	12.063
0.728	0.898	10.0	11.841
0.898	1.068	8.0	9.792
1.068	1.238	11.0	6.822
1.238	.	6.0	7.211
		74.000	74.000

Chi-square test statistic = 5.212735 df = 5 p-value = 0.390473

FITTED DISTRIBUTION



Kolmogorov-Smirnov test statistic = 0.060037 Lilliefors Probability (2-tail) = 0.704131
 Shapiro-Wilk test statistic for normality = 0.976343 p-value = 0.179198

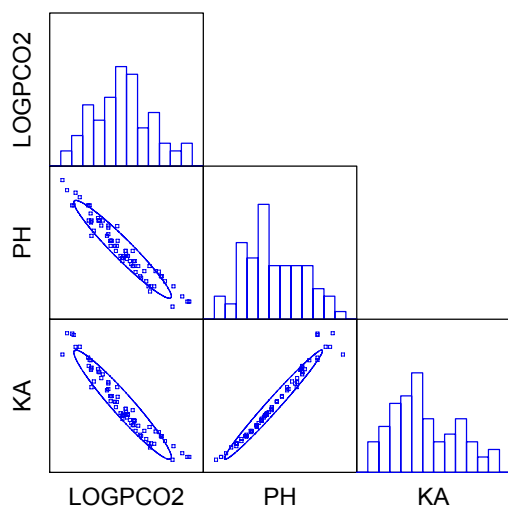
Obviously, the PH and CO₂ are highly correlated. Since the K_A is derived from both it should be correlated to both.

Pearson correlation matrix

	LOGPCO2	PH	KA
LOGPCO2	1.000		
PH	-0.959	1.000	
KA	-0.958	0.985	1.000

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Bartlett Chi-square statistic: 434.381 df=3 Prob= 0.000
 Matrix of Bonferroni Probabilities

	LOGPCO2	PH	KA
LOGPCO2	0.000		
PH	0.000	0.000	
KA	0.000	0.000	0.000

Number of observations: 74

To calculate the K_D values, multiply the K_A by the surface area of the sample. Effective surface areas for the alluvium range from 0.9 to 12.1 m²/g and are normally distributed. There is a positive correlation between clay content and surface area. I would propose that the upper end be used for the fine-grained sediments and the lower end be used for the coarse-grained facies, with some overlap between the two.

The well data and K_A calculations are provided in the two accompanying spreadsheets for your information.

My feeling at this point is that the spatial distribution of the chemistry may not be well defined, so that a simpler application of the mean and variance of the sorption values is warranted. The sorption values are derived by multiplying the K_A values times the effective surface area for each sample. Since the surface area is defined by a distribution, you would have to apply that variance to the process. The surface area distribution (above) has been defined for all samples but has not been defined/analyzed according to grain size variations.

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19-Apr-11
 FOR CLOSEOUT.

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