PROJECT NAME	**907BRI**	Date	28/03/2011
PROJECT NO:	**GEO / 16683**	Approved	Simon Burke
		Page	1 of 1

Sample details					Classification Tests					Density Tests		Undrained Triaxial Compression Tests			Chemical Tests			
Borehole No.	Depth (m)	No.	Type	Description	MC (%)	LL (%)	PL (%)	PI	<425 mic (%)	Bulk (Mg/m³)	Dry (Mg/m³)	Cell Pressure (kPa)	Deviator Stress (kPa)	Shear Stress (kPa)	pH	2:1 W/S SO4 (g/l)	Ground Water SO4 (g/l)	Other tests and comments
TB66	-	-	B	Grey silty CLAY	42					1.74	1.23							Particle Density = 2.65 Mg/m³ Triaxial Permeability Test 4.5kg Compaction Test
TB67	-	-	B	Grey silty CLAY	41					1.71	1.21							Particle Density = 2.65 Mg/m³ Triaxial Permeability Test 4.5kg Compaction Test
TB70	-	-	B	Grey silty CLAY	45					1.99	1.37							Particle Density = 2.69 Mg/m³ Triaxial Permeability Test 4.5kg Compaction Test
TB80	-	-	B	Grey silty CLAY with rare fine gravel	47					1.71	1.16							Particle Density = 2.67 Mg/m³ Triaxial Permeability Test 4.5kg Compaction Test

SUMMARY OF GEOTECHNICAL TESTING

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BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP: TB66 Sample No: Depth:	Description: Firm grey silty CLAY

SPECIMEN DETAILS	
Depth within original sample	
Orientation within original	
Specimen preparation	Remoulded @ NMC with a compactive effort of 4.5kg

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.4	103.4
Height	*mm*	115.5	114.5
Moisture Content	*%*	43	43
Bulk Density	*Mg/m³*	1.77	1.82
Dry Density	*Mg/m³*	1.24	1.27

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	0.84	0.95

CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	25.6

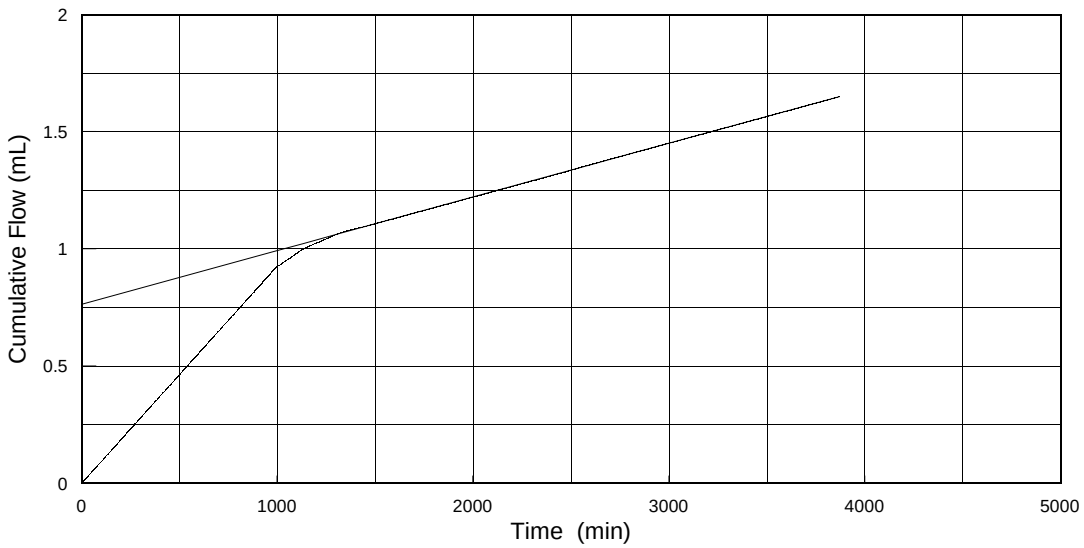
PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC =

5.1×10^{-11} m/s

TEST DURATIONS		
Saturation	*days*	3
Consolidation	*days*	7
Flow	*days*	3

Hydraulic Gradient : 8.9



Checked and Approved	Project Number:	
Initials: PTH	**GEO /16683**	
Date: 28/03/11	Project Name: **VERTASE**	

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BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP: Sample No: TB67 Depth:	Description: Firm grey CLAY lumps with rare fine to medium gravel

SPECIMEN DETAILS	
Depth within original sample	N/A
Orientation within original	Vertical
Specimen preparation	Remoulded @ NMC using a compactive effort of 4.5kg

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.9	104.1
Height	*mm*	114.8	114.0
Moisture Content	*%*	34	36
Bulk Density	*Mg/m³*	1.93	2.00
Dry Density	*Mg/m³*	1.44	1.47

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	0.20	0.99

CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	21.5

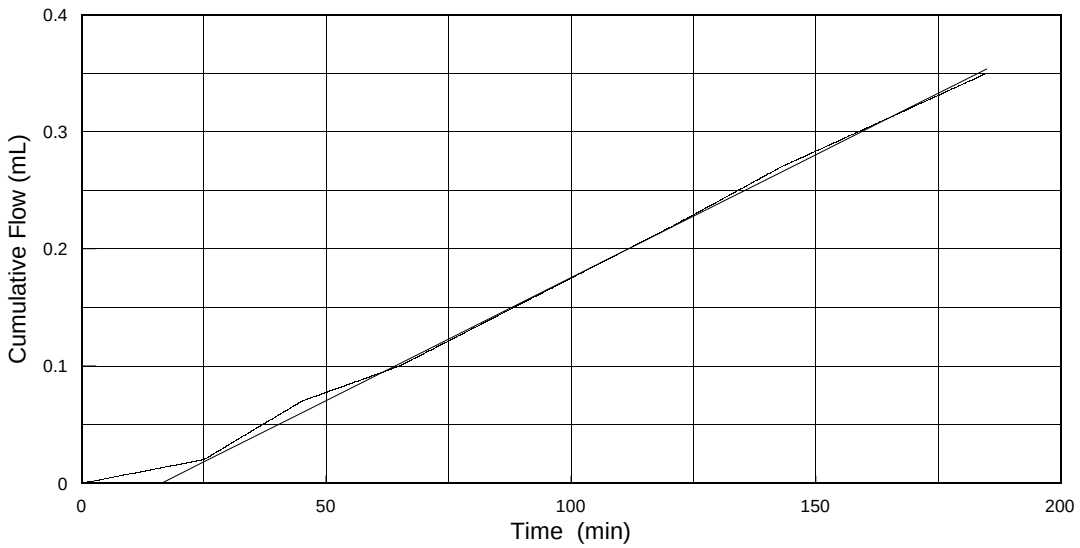
PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC =

4.6×10^{-10} m/s

TEST DURATIONS		
Saturation	*days*	5
Consolidation	*days*	2
Flow	*days*	1

Hydraulic Gradient : 8.9



Checked and Approved	Project Number:	
Initials: PTH	**GEO /16801**	
Date: 11/05/11	Project Name: **Hauxton 907BRI** **Schedule 5**	

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BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP: TB67 Sample No: Depth:	Description: Firm grey silty CLAY

SPECIMEN DETAILS	
Depth within original sample	N/A
Orientation within original	Vertical
Specimen preparation	remoulded @ NMC with a compactive effort of 4.5kg

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.4	103.4
Height	*mm*	115.2	114.2
Moisture Content	*%*	42	42
Bulk Density	*Mg/m³*	1.78	1.84
Dry Density	*Mg/m³*	1.26	1.29

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	0.77	0.98

CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	26.0

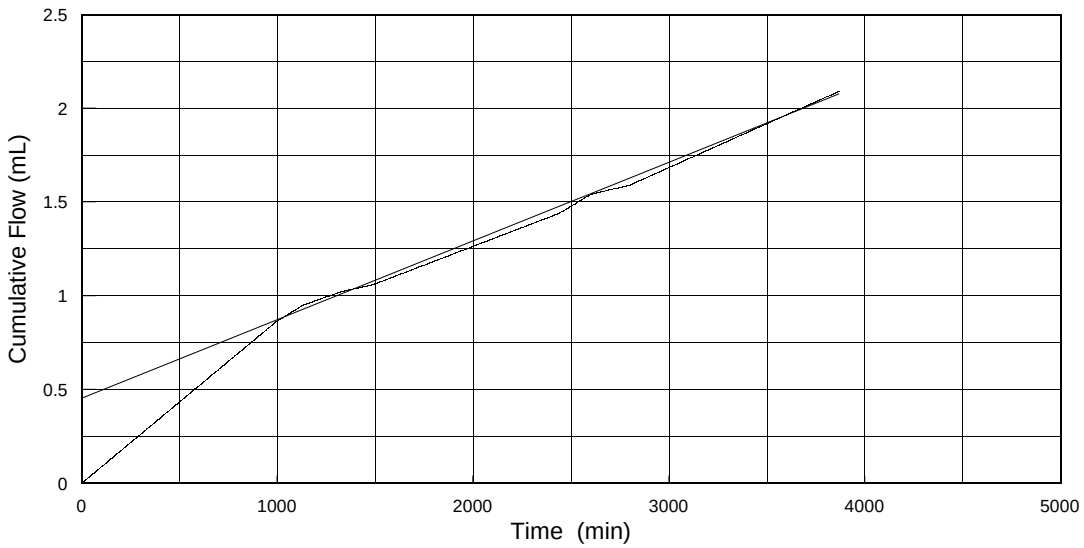
PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC =

9.3×10^{-11} m/s

TEST DURATIONS		
Saturation	*days*	3
Consolidation	*days*	7
Flow	*days*	3

Hydraulic Gradient : 8.9



Checked and Approved Initials: PTH Date: 28/03/11	Project Number: **GEO /16683** Project Name: **VERTASE**	GEOLABS®

BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP: TB70 Sample No: Depth:	Description: Firm grey silty CLAY

SPECIMEN DETAILS	
Depth within original sample	N/A
Orientation within original	Vertical
Specimen preparation	Remoulded @ NMC using a compactive effort of 4.5kg

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.3	103.7
Height	*mm*	114.9	114.2
Moisture Content	*%*	43	43
Bulk Density	*Mg/m³*	1.78	1.80
Dry Density	*Mg/m³*	1.24	1.27

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	0.77	0.98

CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	18.2

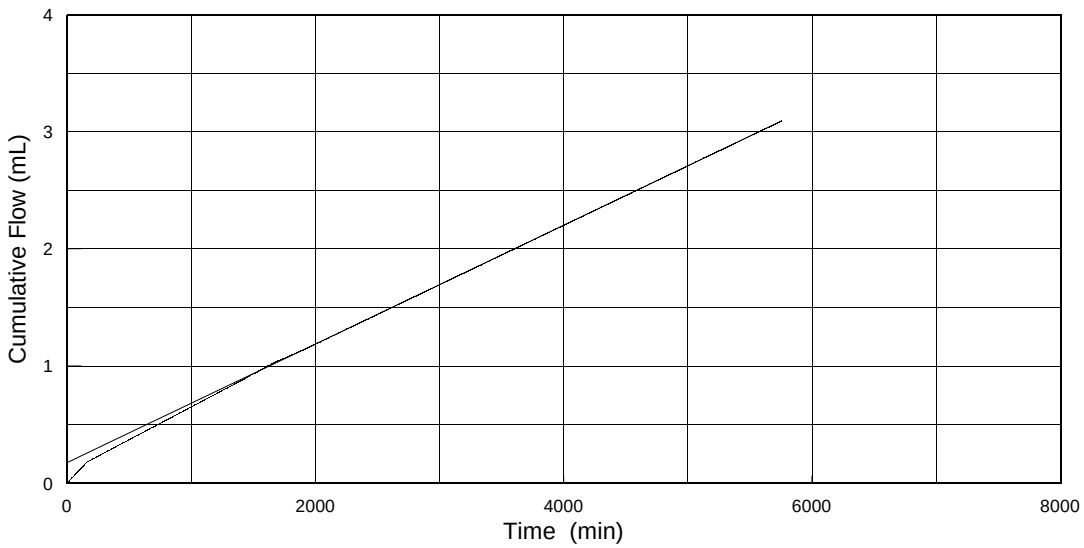
PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC =

1.1×10^{-10} m/s

TEST DURATIONS		
Saturation	*days*	3
Consolidation	*days*	7
Flow	*days*	3

Hydraulic Gradient : 8.9



Checked and Approved	Project Number:	
Initials: PTH	**GEO /16683**	
Date: 30/03/11	Project Name: **VERTASE**	

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BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP: Sample No: TB77 Depth:	Description: Very stiff grey CLAY LUMPS with occasional fine to medium gravel

SPECIMEN DETAILS	
Depth within original sample	N/A
Orientation within original	N/A
Specimen preparation	Remoulded at NMC using a 4.5kg effort

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.7	101.1
Height	*mm*	115.4	111.6
Moisture Content	*%*	23	30
Bulk Density	*Mg/m³*	2.02	2.38
Dry Density	*Mg/m³*	1.65	1.83

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	0.15	0.95

CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	98.3

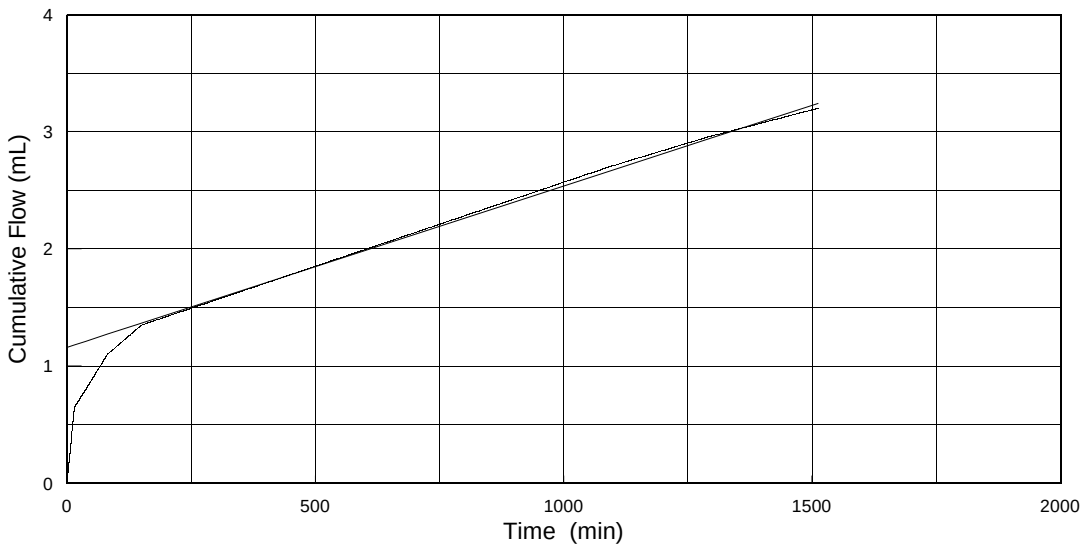
PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC =

3.1×10^{-10} m/s

TEST DURATIONS		
Saturation	*days*	4
Consolidation	*days*	1
Flow	*days*	2

Hydraulic Gradient : 9.1



Checked and Approved	Project Number:	
Initials: PTH	**GEO / 16801**	
Date: 09/05/11	Project Name: **HAUXTON 907BRI** **Scheule 5**	

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BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP:	Description:
Sample No: TB79	Grey slightly silty CLAY with rare brown pockets
Depth:	

SPECIMEN DETAILS	
Depth within original sample	N/A
Orientation within original	N/A
Specimen preparation	Remoulded using 4.5kg effort at natural moisture content

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.2	103.8
Height	*mm*	115.1	114.7
Moisture Content	*%*	39	41
Bulk Density	*Mg/m³*	1.83	1.88
Dry Density	*Mg/m³*	1.32	1.33

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	1.02	0.94

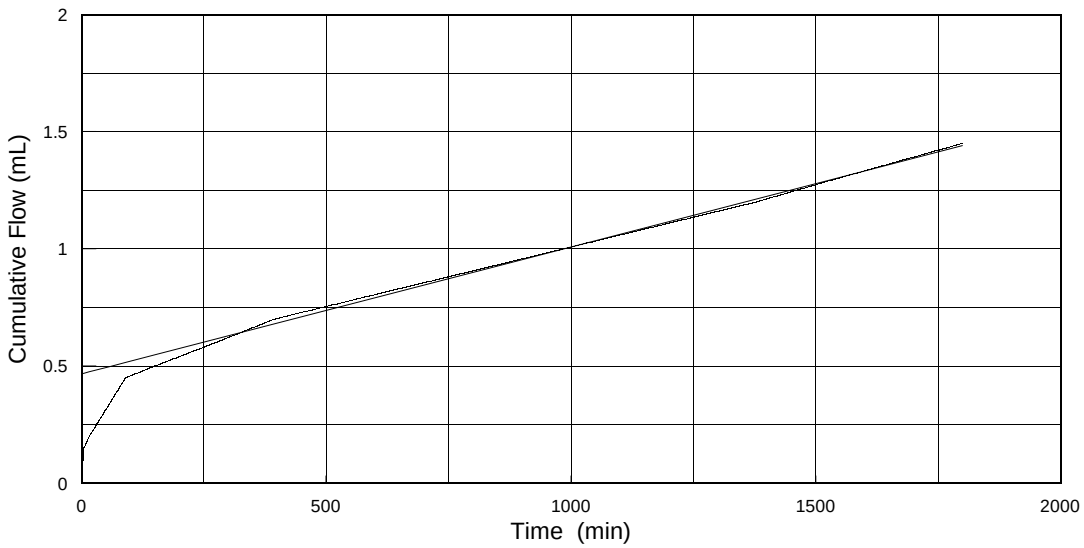
CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	11.4

PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC = 1.2×10^{-10} m/s

TEST DURATIONS		
Saturation	*days*	2
Consolidation	*days*	2
Flow	*days*	2

Hydraulic Gradient : 8.9



Checked and Approved	Project Number:	
Initials: PTH	**GEO / 16801**	
Date: 09/05/11	Project Name: **HAUXTON 907BRI** **Schedule 5**	

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BS1377 : Part 6 : Clause 6 :1990

Determination of Permeability in a Triaxial Cell

Borehole / TP: TB80 Sample No: Depth:	Description: Firm grey slightly silty CLAY

SPECIMEN DETAILS	
Depth within original sample	N/A
Orientation within original	Vertical
Specimen preparation	Remoulded @ NMC using a compactive effort of 4.5kg

TEST DETAILS			
Cell Preparation		Performed in accordance with Clause 3.5	
		INITIAL	FINAL
Diameter	*mm*	104.4	102.9
Height	*mm*	113.9	112.3
Moisture Content	*%*	47	45
Bulk Density	*Mg/m³*	1.74	1.80
Dry Density	*Mg/m³*	1.19	1.24

SATURATION STAGE		
Saturation initially by constant moisture content, followed by back-pressure assistance using 5-10 kPa differential		
'B' value	0.84	0.97

CONSOLIDATION STAGE		
Effective pressure	*kPa*	50
Volume change	*mL*	41.4

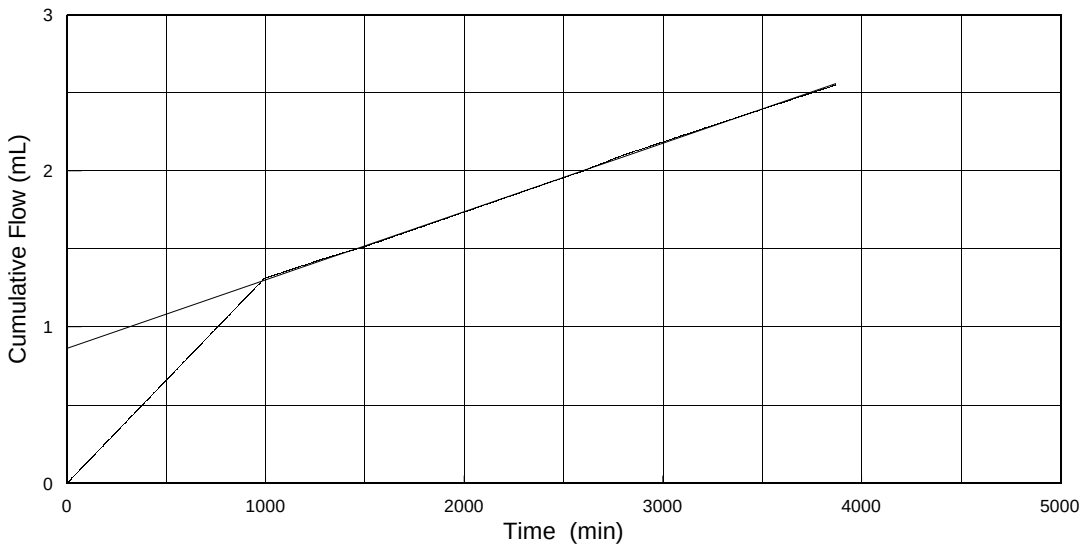
PERMEABILITY STAGE		
Pressure difference across specimen		10
Mean effective stress	*kPa*	45

Coefficient of permeability at 20ºC =

9.7×10^{-11} m/s

TEST DURATIONS		
Saturation	*days*	3
Consolidation	*days*	7
Flow	*days*	3

Hydraulic Gradient : 9.1



Checked and Approved	Project Number:	
Initials: PTH	**GEO /16683**	
Date: 28/03/11	Project Name: **VERTASE**	

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BS1377 : Part 2 : Clause 9 : 1990

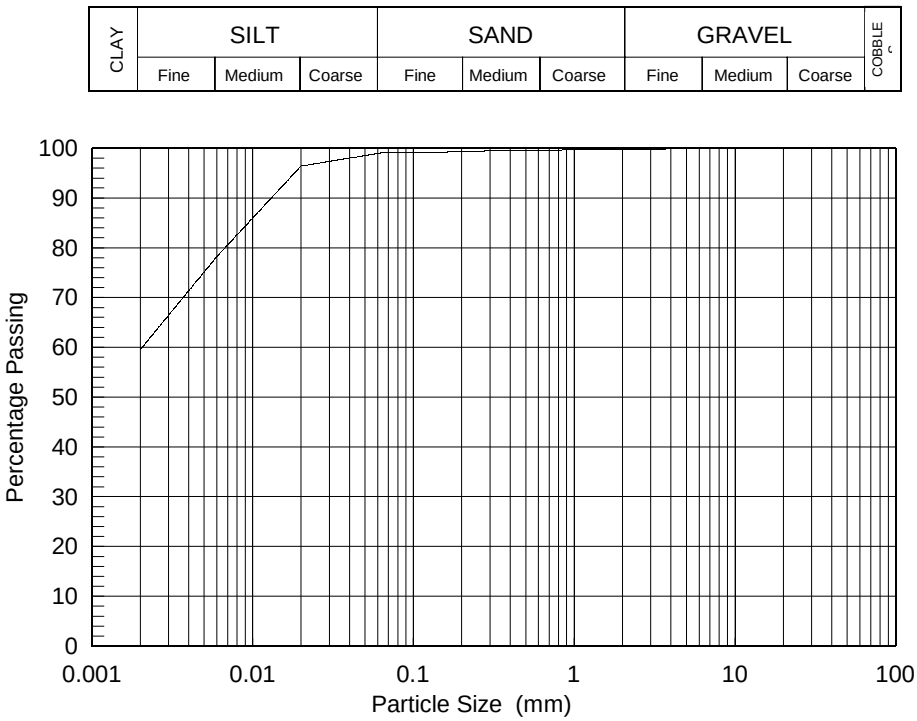
Determination of Particle Size Distribution

Borehole Number: TB66	Description: Grey silty CLAY

BS1377 : Part 2 : Clause 9.2 : 1990 Wet Sieving Method

BS1377 : Part 2 : Clause 9.4 : 1990 Sedimentation by the Pipette Method

SIEVE	
Sieve	% pass
200 mm	100
125 mm	100
90 mm	100
75 mm	100
63 mm	100
50 mm	100
37.5 mm	100
28 mm	100
20 mm	100
14 mm	100
10 mm	100
6.3 mm	100
5 mm	100
3.35 mm	100
2 mm	100
1.18 mm	100
600 µm	100
425 µm	100
300 µm	99
212 µm	99
150 µm	99
63 µm	99



Particle Proportions		
Cobbles	0.0	%
Gravel	0.2	%
Sand	0.7	%
Silt	39.5	%
Clay	59.5	%

PIPETTE	
Particle size	% pass
20.0 µm	96
6.0 µm	78
2.0 µm	60
Preparation: No Pre-treatment used	

Temp (°C)	20

Checked and Approved	Project Number: GEO / 16683	
Initials: SB	Project Name: 907BRI	
Date: 28/03/2011		

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Client: Vertase FLI Limited, Number One, Middle Bridge Business Park, Bristol Road, Portishead BS20 6PN

BS1377 : Part 2 : Clause 9 : 1990

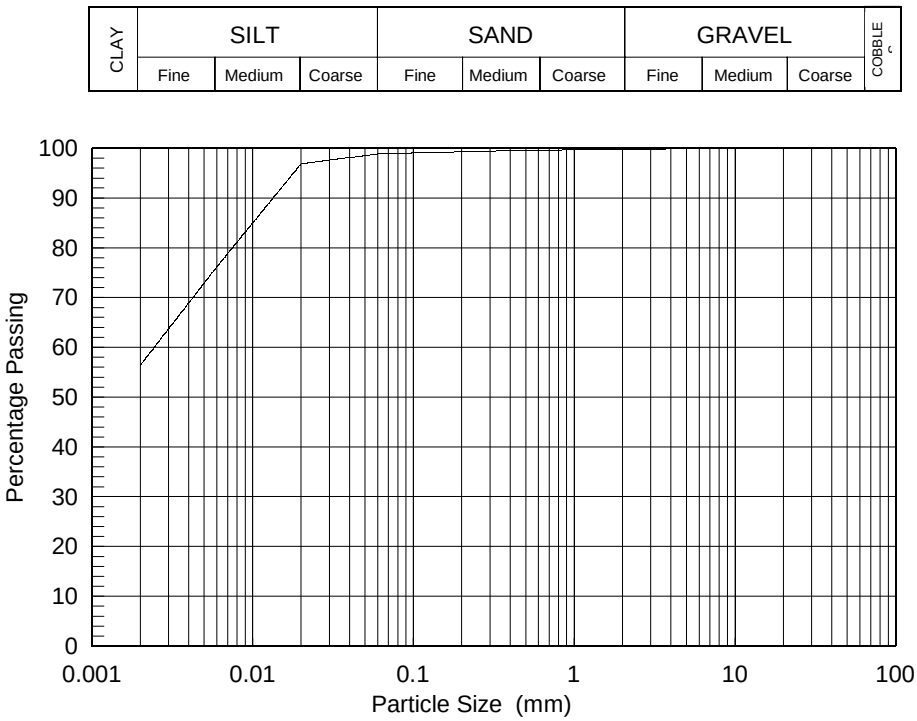
Determination of Particle Size Distribution

Borehole Number: TB67	Description: Grey silty CLAY

BS1377 : Part 2 : Clause 9.2 : 1990 Wet Sieving Method

BS1377 : Part 2 : Clause 9.4 : 1990 Sedimentation by the Pipette Method

SIEVE	
Sieve	% pass
200 mm	100
125 mm	100
90 mm	100
75 mm	100
63 mm	100
50 mm	100
37.5 mm	100
28 mm	100
20 mm	100
14 mm	100
10 mm	100
6.3 mm	100
5 mm	100
3.35 mm	100
2 mm	100
1.18 mm	100
600 µm	100
425 µm	100
300 µm	99
212 µm	99
150 µm	99
63 µm	99



Particle Proportions		
Cobbles	0.0	%
Gravel	0.2	%
Sand	0.8	%
Silt	42.6	%
Clay	56.4	%

PIPETTE	
Particle size	% pass
20.0 µm	97
6.0 µm	76
2.0 µm	56
Preparation: No Pre-treatment used	

Temp (°C)	20

Checked and Approved

Initials: SB

Date: 28/03/2011

Project Number: **GEO / 16683**

Project Name: **907BRI**

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Client: Vertase FLI Limited, Number One, Middle Bridge Business Park, Bristol Road, Portishead BS20 6PN

BS1377 : Part 2 : Clause 9 : 1990

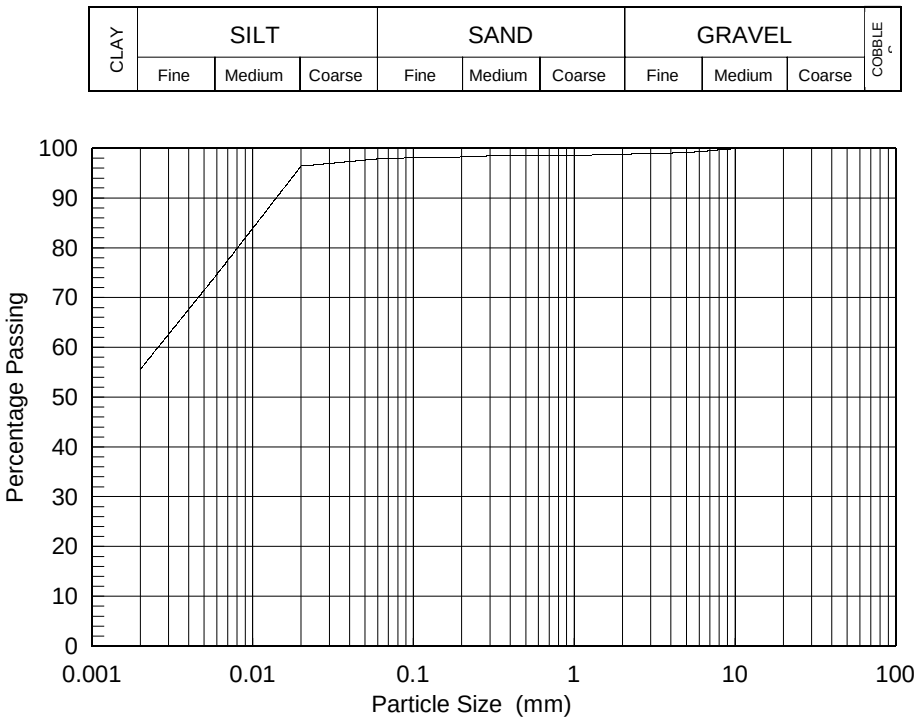
Determination of Particle Size Distribution

Borehole Number: TB70	Description: Grey silty CLAY

BS1377 : Part 2 : Clause 9.2 : 1990 Wet Sieving Method

BS1377 : Part 2 : Clause 9.4 : 1990 Sedimentation by the Pipette Method

SIEVE	
Sieve	% pass
200 mm	100
125 mm	100
90 mm	100
75 mm	100
63 mm	100
50 mm	100
37.5 mm	100
28 mm	100
20 mm	100
14 mm	100
10 mm	100
6.3 mm	99
5 mm	99
3.35 mm	99
2 mm	99
1.18 mm	99
600 µm	99
425 µm	99
300 µm	98
212 µm	98
150 µm	98
63 µm	98



Particle Proportions		
Cobbles	0.0	%
Gravel	1.2	%
Sand	0.9	%
Silt	42.3	%
Clay	55.6	%

PIPETTE	
Particle size	% pass
20.0 µm	96
6.0 µm	75
2.0 µm	56
Preparation: No Pre-treatment used	

Temp (°C)	20

Checked and Approved

Initials: SB

Date: 28/03/2011

Project Number: **GEO / 16683**

Project Name: **907BRI**

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Client: Vertase FLI Limited, Number One, Middle Bridge Business Park, Bristol Road, Portishead BS20 6PN

BS1377 : Part 2 : Clause 9 : 1990

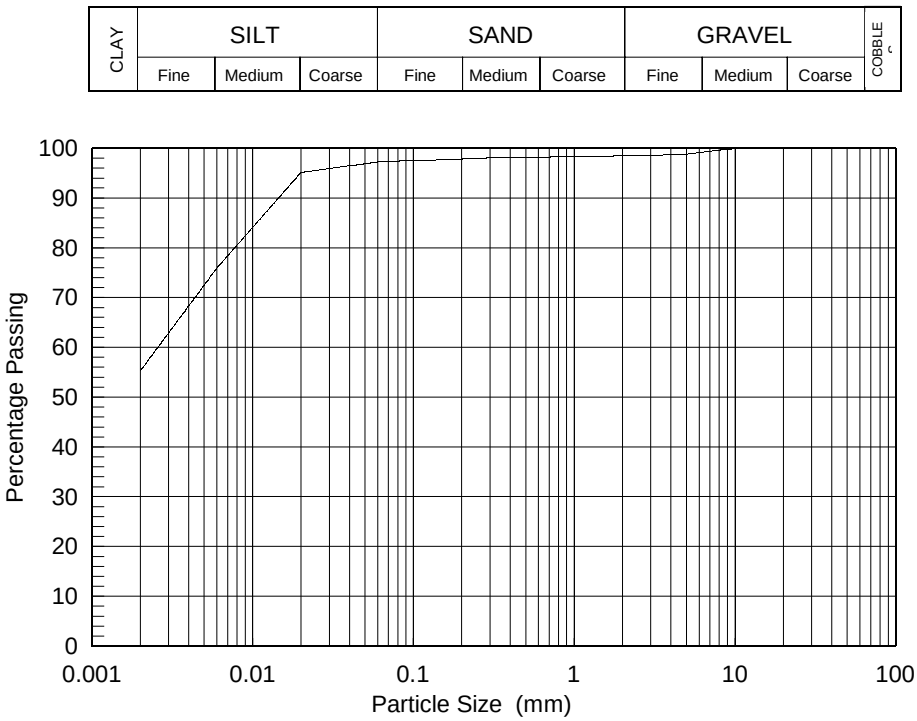
Determination of Particle Size Distribution

Borehole Number: TB80	Description: Grey silty CLAY with rare fine gravel

BS1377 : Part 2 : Clause 9.2 : 1990 Wet Sieving Method

BS1377 : Part 2 : Clause 9.4 : 1990 Sedimentation by the Pipette Method

SIEVE	
Sieve	% pass
200 mm	100
125 mm	100
90 mm	100
75 mm	100
63 mm	100
50 mm	100
37.5 mm	100
28 mm	100
20 mm	100
14 mm	100
10 mm	100
6.3 mm	99
5 mm	99
3.35 mm	99
2 mm	98
1.18 mm	98
600 µm	98
425 µm	98
300 µm	98
212 µm	98
150 µm	98
63 µm	97



Particle Proportions		
Cobbles	0.0	%
Gravel	1.5	%
Sand	1.1	%
Silt	42.1	%
Clay	55.3	%

PIPETTE	
Particle size	% pass
20.0 µm	95
6.0 µm	76
2.0 µm	55
Preparation: No Pre-treatment used	

Temp (°C)	20

Checked and Approved	Project Number: GEO / 16683	
Initials: SB	Project Name: 907BRI	
Date: 28/03/2011		

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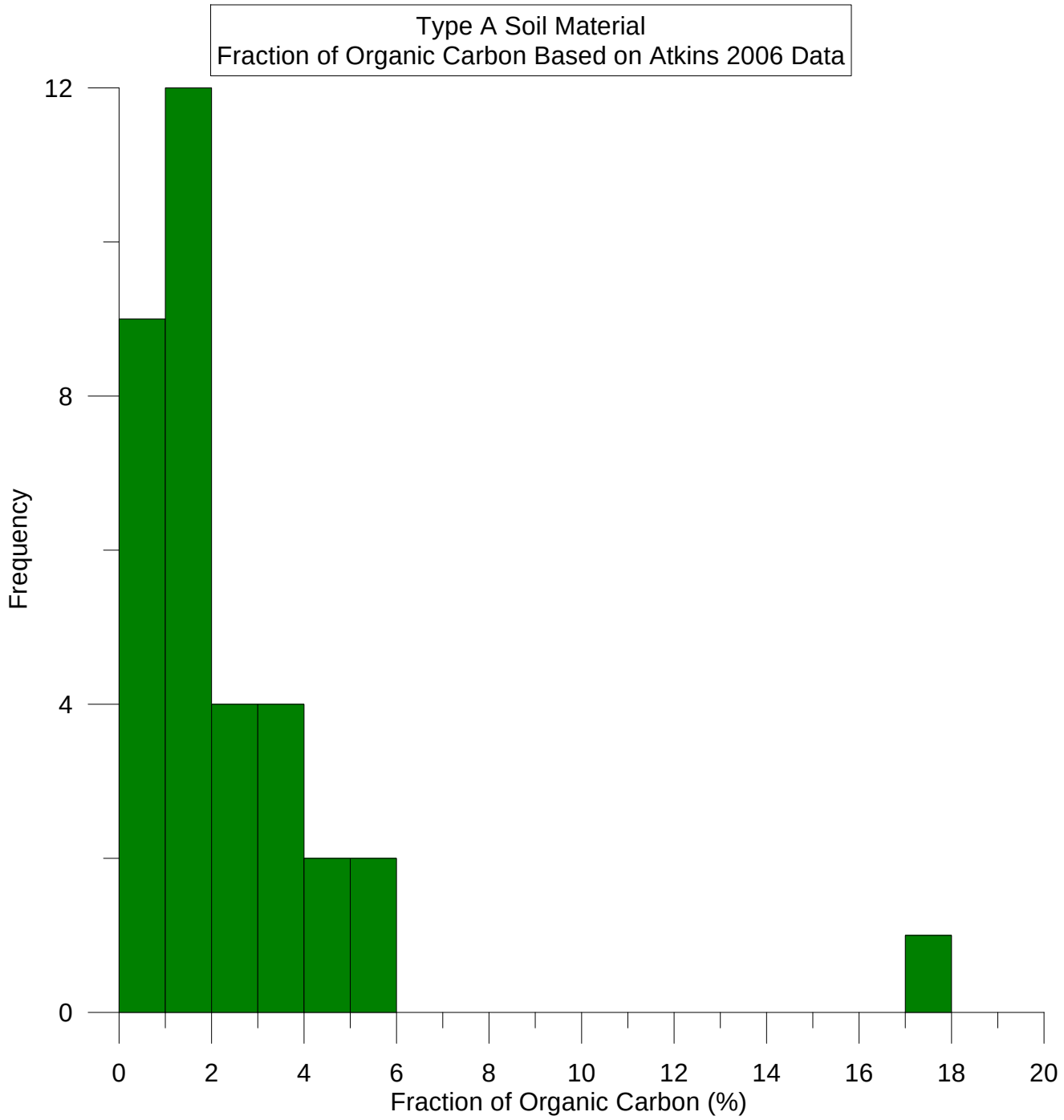
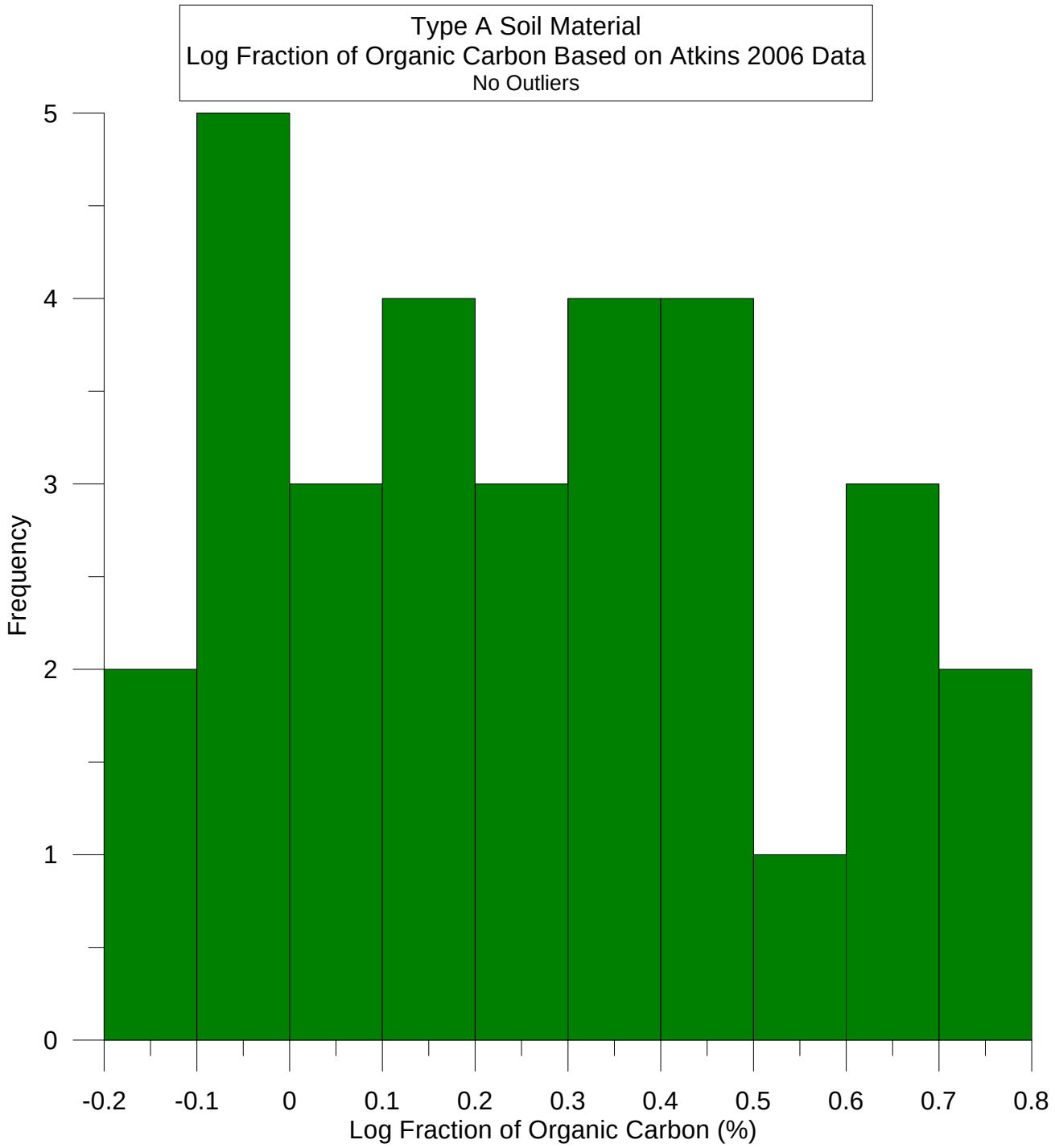
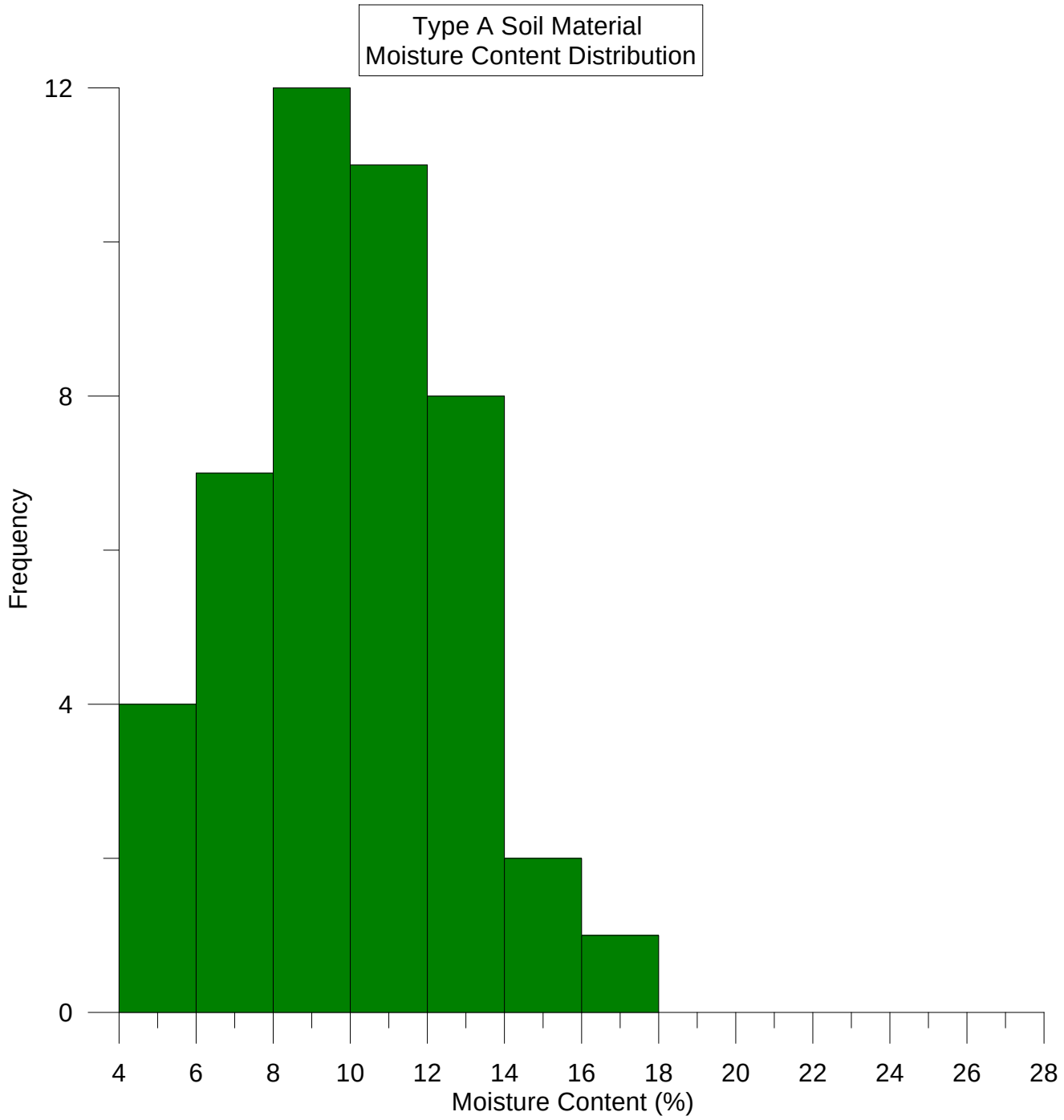
APPENDIX E

SOIL SOURCE PARAMETER SUPPORTING DATA


Type A Soil Material
Fraction of Organic Carbon Based on Atkins 2006 Data
Frequency
0
4
8
12
0
2
4
6
8
10
12
14
16
18
20
Fraction of Organic Carbon (%)

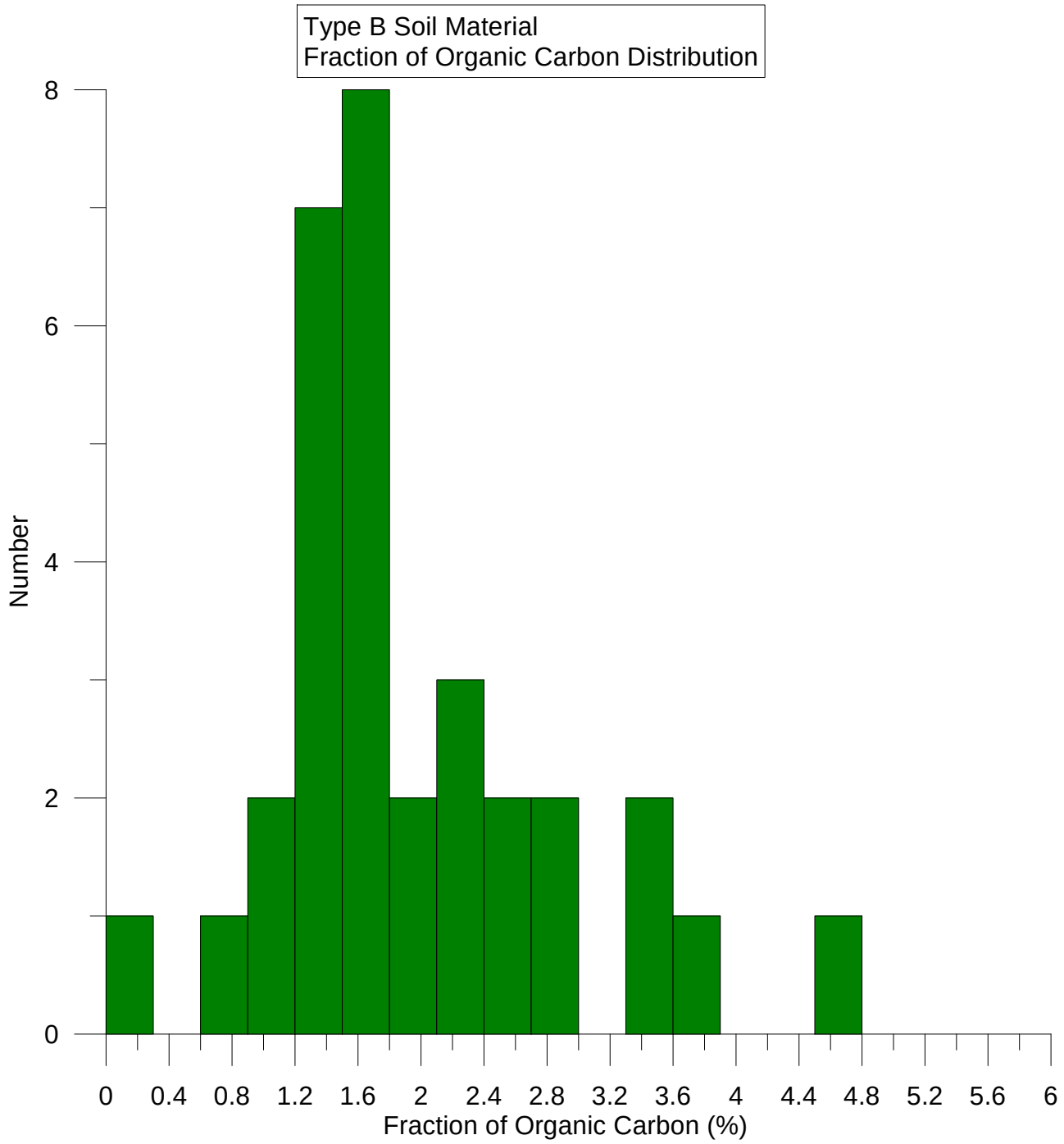

Type A Soil Material
Log Fraction of Organic Carbon Based on Atkins 2006 Data
No Outliers
Frequency
0
1
2
3
4
5
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Log Fraction of Organic Carbon (%)

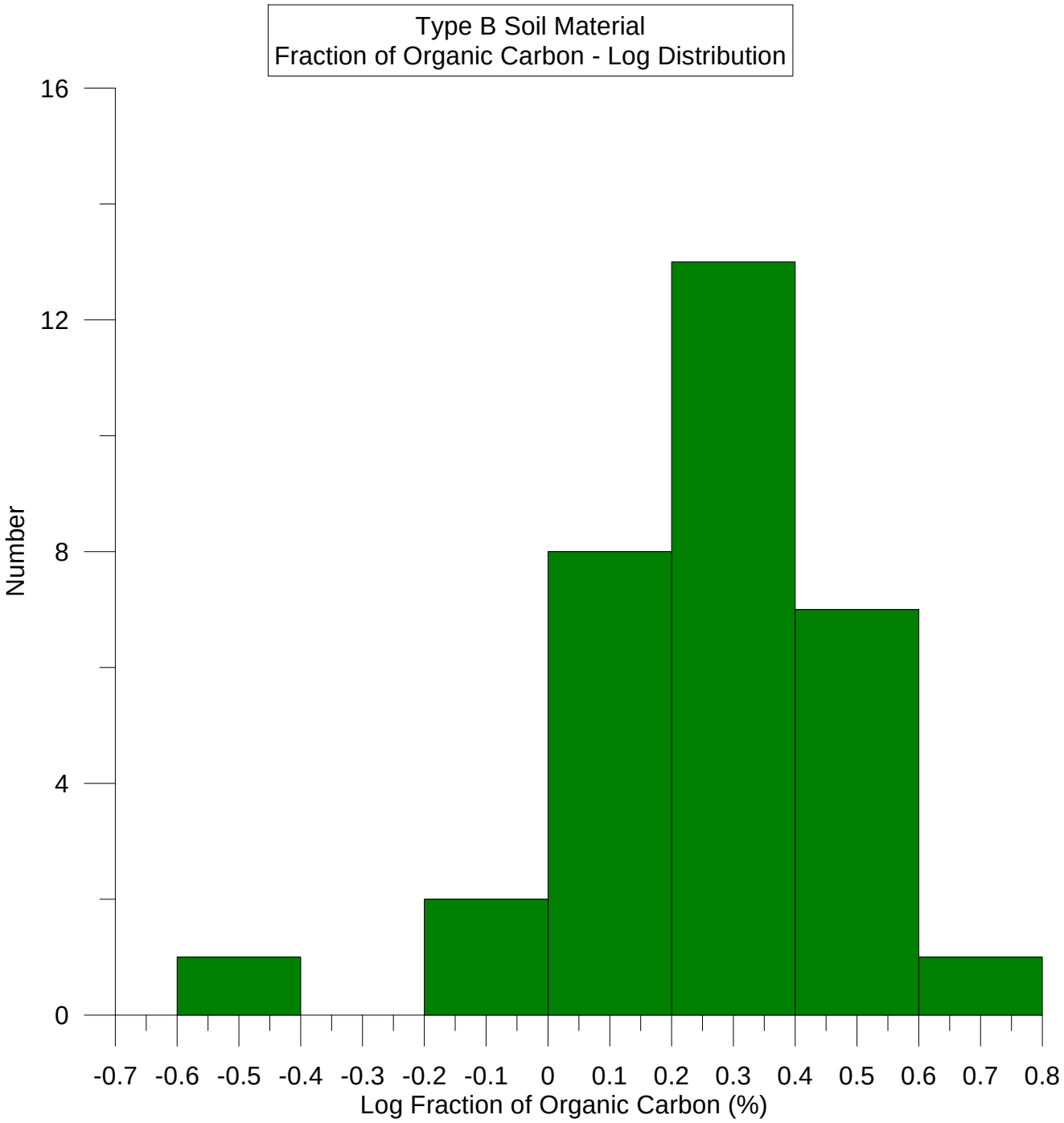

Type A Soil Material
Moisture Content Distribution
Frequency
0
4
8
12
4
6
8
10
12
14
16
18
20
22
24
26
28
Moisture Content (%)

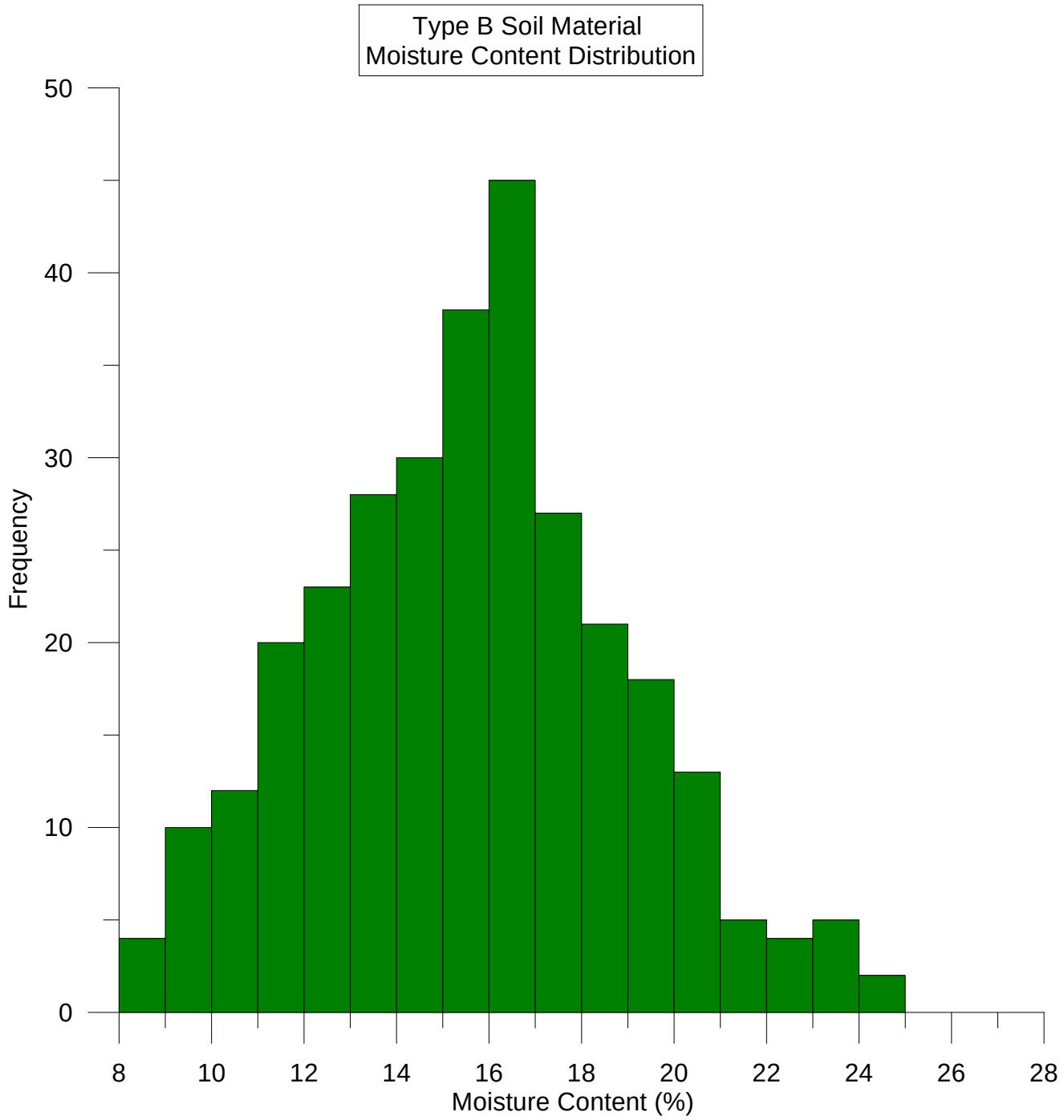
Recorded Fraction of Organic Cabon in Type B Material

Remediati	Fraction of Organic Carbon Values (%)			
TB49	3			
TB50	3.8			
TB55	2.3			
TB57	0.75	4.8		
TB63	3.4			
TB64	1.3	1.5		
TB65	1.4	1.7		
TB83	2.1	1.8	1.3	2.4
TB86	1.7	1.4		
TB95	1	1.3		
TB108	1.3			
TB117	1.6	1.1		
TB118	1.9	2.6	1.8	1.6
TB119	1.7	1.8		
TB135	2.6	2.9		
TB136	3.3	2.4	0.28	

Maximum	4.8
Minimum	0.28
Mean Valu	1.994688
GeoMean	1.772753


Type B Soil Material
Fraction of Organic Carbon Distribution
Number
0
2
4
6
8
0
0.4
0.8
1.2
1.6
2
2.4
2.8
3.2
3.6
4
4.4
4.8
5.2
5.6
6
Fraction of Organic Carbon (%)


Type B Soil Material
Fraction of Organic Carbon - Log Distribution
Number
16
12
8
4
0
-0.7
-0.6
-0.5
-0.4
-0.3
-0.2
-0.1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Log Fraction of Organic Carbon (%)


Type B Soil Material
Moisture Content Distribution
Frequency
0
10
20
30
40
50
8
10
12
14
16
18
20
22
24
26
28
Moisture Content (%)

APPENDIX F

CONTAMINANT OF CONCERN – INPUT VALUE JUSTIFICATIONS

References Used to Obtain Physical-Chemical Properties of Priority Organic Contaminants

1. Physical – Chemical Properties and Environmental Fate for Organic Chemicals, 2nd Edition, Mackay *et al*, 2006;
2. Compilation of data for priority organic pollutants for derivation of Soil Guideline Values, Science Report SC050021/SR7, Environment Agency, 2008;
3. ChemIDplus – http://chem.sis.nlm.gov/chemicals, United States National Library of Medicine, accessed April 2011;
4. Pesticide Properties Database – www.ars.usda.gov, United States Department of Agricultural Research Services, October 2001;
5. Toxnet Hazardous Substances Database - http://toxnet.nlm.nih.gov – accessed April 2011;
6. Technical Support Document for the Hazardous Waste Identification Rule: Risk Assessment for Human and Ecological Receptors – Volume 1, Appendix A, US Environmental Protection Agency, Office of Solid Waste, August 1995;
7. Site Screening Guidance: Technical Background Document Part 5, Chemical Specific Parameters, Report EPA/540/R-95/128, United States Environmental Protection Agency, July 1996;
8. RCRA Delisting Technical Support Document – Appendix A Chemical Specific Data, United States Environmental Protection Agency, RCRA Delisting Team, October 2008;
9. Review Report for the Active Substance Ethofumesate, SANCO/6503/VI/99-final, European Commission Health and Consumer Protection Directorate-General, May 2002;
10. Screening Information Dataset – Cyclohexanone, Identifiers, Physical and Chemical Properties, Organisation for Economic Co-Operation and Development, 2002
11. Screening Information Dataset – 4-Chloro-o-cresol, Identifiers, Physical and Chemical Properties, Organisation for Economic Co-Operation and Development, EINECS-No.: 216-381-3, 1998.
12. A review of mecoprop attenuation in the subsurface, S.R Buss, J Thrasher, P Morgan, *et al*, Quarterly Journal of Engineering Geology and Hydrogeology, 2006.

1,2 Dichloroethane – CAS 107-06-2

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (11.48,76)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Normal (0.049) standard deviation of 0.025)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform (400 – 720) anaerobic degradation in natural waters (most conservative values)	1
Maximum Solubility (mg/l)	Uniform (8520,8680)	2,7

Justification

K_{oc} –16 values were obtained from the references. For the probability distribution function, it is proposed to use the uniform range 11.48 to 76, conservatively discounting the value of 151.356 as it an order of magnitude greater than all other quoted values.

Henry's Law constant (dimensionless) – Reference 1 gives 26 values of Henry's Law constant from 0.07471 to 0.1286, with a mean value of 0.049. Of these values the upper value 0.1286 is an order of magnitude higher than all other values and has therefore been conservatively discounted. Values quoted from References 2 and 3 and 8 give values of 0.0482, 0.0488 and 0.0401 respectively, all similar to the average value from Reference 1. Based on the histogram for values, a normal distribution was selected with an average value of 0.049 with a standard deviation of 0.0245.

Half Life – The most conservative values quoted in Reference 1 were for biodegradation in water was 400 to 720 days in anaerobic conditions.

Solubility – Using a uniform distribution between the values given in references 2 and 8.

Dicamba – CAS 1918-00-9

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	LogTriangular (0.1,2.5,42.65)	1,4
Henry's Law Constant (dimensionless)	Uniform(8.87e-9,8.91e-8)	1,3,4
Half Life (days) in groundwater	Uniform (151 – 443)	1
Maximum Solubility (mg/l)	Single (8310)	3,4

Justification

K_{oc} – 34 values were provided by the listed references. Typically, the values were in the range 0.1 to 42.65 with two values from Mackay significantly outside the range (120 and 460 ml/g) which were discounted. Based on the histogram of the log K_{oc} values, a log triangular distribution was considered most appropriate with a midpoint of 2.5 ml/g.

Henry's Law Constant – 9 values were obtained from the references. Of these two values from Reference 1 (3.7e-5 and 1e-5) were 3 to 4 orders of magnitude greater than the other values and therefore discounted from the distribution. For the remaining values, a uniform distribution was considered most appropriate.

Half Life – Reference 1 gives a range of half lives in groundwater from 14 to 443 days. However, another value quoted gives a half life of 151 days at 12 ^{o}C which is more representative of anticipated groundwater temperatures. Therefore, a conservative range of 151 to 443 days has been used in the model.

Solubility – The solubility of 8310 mg/l was quoted in the two sources listed above.

Schradan (Octamethylpyrophosphoramide) – CAS 152-16-9

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Loguniform (0.31,7)	5,8
Henry's Law Constant (dimensionless)	Loguniform (2.58e-15,1.55e-8)	5,6,8
Half Life (days) in groundwater	Uniform (1825 – 3650)	No data, conservative assumption of 5 to 10 years
Maximum Solubility (mg/l)	Single (1e6)	5,6,8

Justification

K_{oc} – Only two values were available. A loguniform distribution was considered appropriate due to the relatively large range of the values.

Henry's Law - Only two values were available. A loguniform distribution was considered appropriate due to the very large range of the values.

Half Life – No data was available on the half life of Schradan. A conservative half life of 5 to 10 years was assumed.

Solubility - The solubility of 1,000,000 mg/l was quoted in the three sources listed above.

Bis(2-chloroethyl)ether – CAS 111-44-4

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform(13.8,76)	1, 6,7,8
Henry's Law Constant (dimensionless)	Uniform(5.34e-4,8.71e-4)	1,3,6,7,8
Half Life (days) in groundwater	Uniform (360,720)	1
Maximum Solubility (mg/l)	Uniform (10200,17200)	1,3,6,7,8

Justification

K_{oc} – Literature values range from 13.8 to 76 ml/g with no obvious pattern, therefore a uniform distribution using the entire range of values has been selected.

Henry's Law Constant – Of the six literature values obtained, all are of the order 1×10^{-4} with the exception of one value (from Reference 1) which was 1.16×10^{-2}. This value was conservatively discounted and a uniform distribution was selected for the other values.

Half life in groundwater – The only data available for half life was taken from reference 1, for biodegradation in water in anaerobic conditions.

Solubility – Values given for solubility were between 1020 and 1720 mg/l, a uniform distribution between was selected.

Ethofumesate – CAS 26225-79-6

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform(97,245)	4,9
Henry's Law Constant (dimensionless)	Loguniform(2,74e-7,1.5e-6)	3,4,9
Half Life (days) in groundwater	Uniform (1825,3650)	No available data
Maximum Solubility (mg/l)	Single (50)	3,4,9

Justification

K_{oc} – Reference 9 gave a range of 97 to 245 ml/g from 11 values with a mean value of 147. Reference 4 gave 5 values from 120 to 760 ml/g. The value of 760 ml/g was significantly higher than all other values and therefore conservatively discounted and a uniform distribution based on the values from Reference 9 was selected.

Henry's Law Constant – Literature values from References 3 and 4 gave a value of 1.5e-6 while reference 9 gave 2.74e-7. Therefore a loguniform distribution between the 2 values was selected.

Half Life in groundwater – No literature values were available, although reference 9 indicated that Ethofumesate is not readily biodegradable. Therefore a conservative half life of 5 to 10 years was assumed.

Solubility – Literature values all quoted a solubility of 50 mg/l.

Trichloroethene – CAS 79-01-6

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Logtriangular(25.12,141,776.24)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Uniform (0.275,0.55)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform (321,1654)	1
Maximum Solubility (mg/l)	Uniform (1180,1370)	1,2,3,6,7,8

Justification

K_{oc} – Values from references 2,3,7 and 8 were typically in the range 94 to 141 ml/g, reference 6 gave a value of 460 mg/l. Thirty six values were given in Reference 1, in the range 25.11 to 776.24 ml/g with the exception of two values greater than 2,500 ml/g.

Discounting the two values greater than 2,500 ml/g, the values fit a log triangular distribution with a mid-point of 141 equal to the Environment Agency recommended value (Reference 2).

Henry's Law Constant –The histogram indicated three populations present in the available data, <0.2, 0.275 to 0.55 and >0.7. Given the values given by the Environment Agency (Reference 2) and the USEPA (6,7 and 8) are all 0.42, the mid-point of the range 0.275 to 0.55 a uniform distribution in this range has been selected.

Half life in Groundwater – Based on Reference 1 values for anaerobic half life in water of Trichloroethene are 321 to 1654 days.

Solubility – Literature values range from 1180 to 1370 mg/l with no clear distribution, therefore a uniform distribution has been used.

Tetrachlorethene – CAS 127-18-4

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular (50,296,500)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Triangular (0.1,0.68,1.21)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform (720,1653)	1
Maximum Solubility (mg/l)	Triangular(200,225,230)	2,3,6,7,8

Justification

K_{oc} – The literature values given in Reference 1 give a very wide range of values from 13.48 to 10,715 ml/g. Other literature values are given as 265, 269 (Environment Agency recommended value) and 420 ml/g.

Based on the histogram of the values, there appears to be several separate distributions of values and the range 50 to 500 was considered most appropriate as it is approximately centred on the recommended Environment Agency value and is more conservative in deriving the soil-water partition coefficient as at lower values less contaminant will sorb to the soil. A triangular distribution was selected with 296 mg/l as the midpoint.

Henry's Law Constant – The histogram of all the available values gives a triangular distribution with the values 0.1, 0.68 and 1.21. The value from Reference 6 (1.59) was discounted as it fell outside the histogram distribution.

Half Life in Groundwater – The quoted values for anaerobic biodegradation in water is between 98 and 1653 days. A more conservative lower value of 720 days was selected based on the maximum aerobic half life in groundwater which is more conservative than the lowest value for the anaerobic half life. Based on the two available values, a uniform distribution was selected.

Solubility – Based on the available literature values for solubility, a triangular distribution was selected with a midpoint of 225 mg/l.

Cis 1,2 Dichloroethene – CAS 156-59-2

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (35.6,69.18)	1,6,7,8
Henry's Law Constant (dimensionless)	Logtriangular (0.129,0.185,0.303)	1,3,6,7,8
Half Life (days) in groundwater	Uniform (720,2875)	1
Maximum Solubility (mg/l)	Uniform (4900,6410)	1,3,6,7,8

Justification

K_{oc} – Only limited literature values were available which ranged between 35.6 and 69.18 ml/g. Therefore, these values were used with a uniform distribution.

Henry's Law Constant – Literature values ranged from 0.129 to 0.956. Three values (0.754, 0.794 and 0.956) were significantly higher than other literature values and therefore conservatively discounted. Based upon the histograms of the literature values a logtriangular PDF was selected with a midpoint of 0.185.

Half Life in Groundwater – Anaerobic biodegradation in water was given as between 112 and 720 days, with the aerobic half life in groundwater 56 – 2875 days. Therefore a uniform distribution was selected based on the most conservative half-lives.

Solubility – Literature values were between 4900 and 6410 mg/l and therefore these values were selected with a uniform distribution.

Vinyl Chloride – CAS 75-01-4

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular (2.99,16.6,57)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Triangular (0.184,1.085,2.29)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform (720,2875)	1
Maximum Solubility (mg/l)	Uniform (2700,2760)	2,3,6,7

Justification

K_{oc} – Available literature values ranged from 2.99 to 57 with no clear distribution. A triangular distribution was selected with a midpoint of the recommended EA (Reference 2) value 16.6 ml/g.

Henry's Law - Fifteen literature values were available between 0.184 and 42.998. Of these values the majority were in the range 0.184 to 2.29 with an average value of 1.15. Four values from 12.6 to 42.998 significantly outside of the range based on data histograms and were therefore conservatively discounted.

A triangular distribution of 0.184, 1.085,3.43 was selected with the EA recommended value (a similar value to the average of the selected distribution) as a midpoint.

Half Life in Groundwater – Values in Reference 1 gave a range of 112 to 720 days for biodegradation half life in aqueous anaerobic conditions, and 56 to 2875 days for half life in groundwater based on aerobic and anaerobic. Therefore a conservative uniform distribution of 720 to 2875 days has been assumed.

Solubility - Literature values ranged from 730 to 8800 mg/l. The most common recommended value was 2700 to 2760 mg/l and this range was selected.

Cylcohexanone – CAS 108-94-1

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (10,66.53)	1,5,10
Henry's Law Constant (dimensionless)	Uniform (3.68e-4, 9.16e-4)	1,3,5,10
Half Life (days) in groundwater	Uniform (1825, 3650)	No available data
Maximum Solubility (mg/l)	Uniform (23000,25000)	1,3,10

Justification

K_{oc} – Three literature values were obtained and a uniform distribution between the minimum and maximum was selected.

Henry's Law Constant – Six values were obtained, one value (2.09e-3) was an order of magnitude greater than all other values and was not included in the selected uniform distribution.

Half Life in Groundwater - No data was available, a conservative half life of 5 to 10 years was selected.

Solubility – Reference 1 gave literature values of 23000 and 93200 mg/l. Values from other sources were 23000 and 25000. A uniform distribution was selected between 23000 and 25000 discounting the value of 93200.

Hempa (Hexamythlphosphoramide) – CAS 680-31-9

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Single (34)	5
Henry's Law Constant (dimensionless)	Single (8.17e-7)	3,5
Half Life (days) in groundwater	Uniform (1825,3650)	No Data available
Maximum Solubility (mg/l)	Uniform (1e6)	3,5

Justification

K_{oc} – Only one value available.

Henry's Law – Only one value available.

Half Life in Groundwater – No data available, conservative assumption of 5 to 10 years.

Solubility - Only one value available.

1,2 Dichlorobenzene – CAS 95-50-1

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular (109,379,891)	1,2,6,7,8
Henry's Law Constant (dimensionless)	LogTriangular(0.049,0.0786,0.151)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform (365,720)	1
Maximum Solubility (mg/l)	Triangular (125,133,156)	2,3,6,7,8

Justification

K_{oc} – The literature values range from 109 to 39,810 ml/g with the majority of values between 109 and 1000 ml/g. The histogram of the data showed a broadly triangular distribution, with most values concentrated between 200 and 450. A triangular distribution was therefore selected with a conservative upper value of 891 and a midpoint of 379, the Environment Agency recommended value in Reference 2.

Henry's Law Constant - The distribution of literature values was predominantly uniform although there was a concentration of values between 0.07 and 0.09. Therefore a triangular distribution was selected with a midpoint of 0.0786 – the EA recommended value (reference 2).

Half Life in Groundwater - A number of half life values in water were reported. Anaerobic biodegradation in water was reported as 120 to 720 days while other sources quoted half lives up to 1 year. Therefore a uniform distribution was selected with the two most conservative values available as the upper and lower limits.

Solubility – Available literature values were between 125 and 156 mg/l. A triangular distribution was selected with the recommended EA value (Reference 2) selected as the midpoint.

2,4,6 Trichlorophenol – CAS 95-50-1

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	LogTriangular (109,1513,6918)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Triangular (5.32e-5,1.176e-4,3.18e-4)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform (169,1820)	1
Maximum Solubility (mg/l)	Triangular (434,750,800)	2,3,6,7,8

Justification

K_{oc} – The available literature values ranged from 109 to 6918 ml/g and based on the histogram of the values would be best represented by a logtriangular distribution. The histogram showed the midpoint to be in the range . A midpoint of 1513 (the EA recommended value (reference 2)) was selected as it in the range of the most commonly occurring values.

Henry's Law – A total of ten literature values were obtained and a triangular distribution selected based on the histogram of the values.

Half Life in Groundwater - Literature values gave a biodegradation half life in anaerobic aqueous conditions of between 169 and 1820 days, in groundwater literature values were 14 (based on aerobic biodegradation) and 1820 (based on anaerobic degradation). A uniform distribution was selected using the most conservative (highest) half life range.

Solubility – Literature values were typically between 750 and 800 mg/l, although the Environment Agency recommended value was 434 mg/l. Therefore a triangular distribution (434,750,800) was selected.

4,6 Dinitro-o-cresol – CAS 534-52-1

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular(100,257,602)	1,4,5
Henry's Law Constant (dimensionless)	Loguniform (5.77e-5, 1.743e-2)	1,3
Half Life (days) in groundwater	Uniform (28,42)	1
Maximum Solubility (mg/l)	Uniform (150,290)	1,3

Justification

K_{oc} – Eleven literature values were obtained for K_{oc}. Of these, 8 values were in the range 100 to 602 with most values in the range 240 to 340. Two values were significantly higher than the majority of the values (1905 and 3715 ml/g) and one value was significantly lower than all other values (23 mg/l). Given the distribution of the values, a triangular PDF was selected with 257 as the midpoint.

Henry's Law Constant – Only three values were available. Given that there was a variation between the values of up to 3 orders of magnitude, a lognormal PDF was selected.

Half Life in Groundwater – The literature values of half life in groundwater in anaerobic conditions ranged between 2.83 and 42 days. Therefore a uniform distribution using the most conservative values was selected.

Solubility – Literature values for solubility ranged from 150 to 290 mg/l with no clear distribution. Therefore a uniform distribution was selected.

4-Chloro-2-methylphenol – CAS 1570-64-5

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (124,700)	5,11
Henry's Law Constant (dimensionless)	Uniform(4.44e-5,5.31e-5)	3,5,11
Half Life (days) in groundwater	Uniform(1825,3650)	No data
Maximum Solubility (mg/l)	Uniform (2300,4000)	3,5,11

Justification

K_{oc} – Six literature values were obtained, of which two were an order of magnitude smaller than the other values. The two lower values were both based upon acidic soils and not considered representative of the site conditions. Based on the remaining four values a uniform distribution was selected.

Henry's Law Constant - Four values of Henry's law constant were identified. Of these, one value was an order of magnitude higher than the other values and conservatively discounted. A uniform distribution was selected based on the other three values.

Half Life in Groundwater – No data was available and a conservative uniform distribution between 5 and 10 years has been assumed.

Solubility - Two values for solubility were obtained and a uniform distribution selected.

Dichloroprop – CAS 120-36-5

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (34,170)	1,4,5
Henry's Law Constant (dimensionless)	Loguniform (1.09e-7,3.6e-4)	1,3,4,5
Half Life (days) in groundwater	Uniform(824,1235)	5
Maximum Solubility (mg/l)	Single (350)	1,3,4,5

Justification

K_{oc} – Twelve literature values were obtained, of which one (1000 ml/g) was discounted due to being at least one order of magnitude above all other values. There was no clear distribution in the remaining values and therefore a uniform distribution was selected.

Henry's Law Constant – Four literature values were obtained which ranged from 1.09×10^{-7} to 3.6×10^{-4}. Due to the wide variation in values a loguniform distribution was selected.

Half Life in Groundwater - The only range of values for anaerobic half life in groundwater was calculated for groundwater at 15 degrees. As only two values were available a uniform distribution was selected.

Solubility - Of the eight literature values obtained, six gave a solubility of 350 mg/l and this was selected as a single input, the other values (50 and 710 mg/l) being discounted.

Dimefox – CAS 115-26-4

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Single(2.2)	5
Henry's Law Constant (dimensionless)	Uniform (8.17e-7,9.12e-7)	3,5
Half Life (days) in groundwater	Uniform(1825,3650)	No data
Maximum Solubility (mg/l)	Single (1e6)	3,5

Justification

K_{oc} – Only one literature value was available and therefore a single distribution has been selected.

Henry's Law Constant - Two values were obtained for the Henry's Law Constant and a uniform distribution between the two values was selected.

Half life in Groundwater – No literature values were available and a conservative uniform distribution between 5 and 10 years was selected.

Solubility – The two literature values obtained both gave a solubility of 1×10^6 mg/l and a single value distribution was therefore selected.

MCPA – CAS 94-74-6

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform(10,154)	1,4,5
Henry's Law Constant (dimensionless)	Uniform (1.96e-8,1.96e-7)	1,3,4,5
Half Life (days) in groundwater	Uniform(20,25)	1
Maximum Solubility (mg/l)	Uniform(630,835)	1,3,4,5

Justification

K_{oc} – Literature values were between 10 and 1862 ml/g. Two values greater than 1,000 ml/g and another of 309 were significantly higher than all other values were conservatively discounted. Based upon the remaining values a uniform distribution was selected.

Henry's Law Constant – Six values were obtained and there was no clear pattern of distribution and therefore a uniform distribution was selected.

Half Life in Groundwater - Only two values were given and a uniform distribution was selected.

Solubility – Thirteen literature values were obtained, of which three were discounted as they were significantly higher than all other values. There was no clear pattern in the remaining solubility values and therefore a uniform distribution was selected.

Mecoprop – CAS 7085-19-0

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (5.3,68)	1,5,12
Henry's Law Constant (dimensionless)	Loguniform (4.48e-9, 7.44e-7)	1,3,5
Half Life (days) in groundwater	Uniform(28,280)	1
Maximum Solubility (mg/l)	Uniform(620,895)	1,3,5,12

Justification

K_{oc} – A uniform distribution was selected as there was no clear pattern in the data. One value (128.825) was conservatively discounted as it was significantly higher than all other values.

Henry's Law Constant – Four literature values were available and due to the wide range of values a loguniform PDF was selected using the highest and lowest literature values.

Half Life in Groundwater - Two ranges were available for anaerobic aqueous biodegradation and biodegradation in groundwater (taking the aerobic and anaerobic half lives). The most conservative range of half lives was selected with a uniform PDF.

Solubility - Three values were available from literature, 620, 734 and 895 mg/l. With no clear distribution, a uniform PDF was selected.

Phenol – CAS 108-95-2

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Uniform (10,46.77)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Uniform (1.29e-5,2.9e-5)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform(8,20)	1
Maximum Solubility (mg/l)	Uniform(82800,91000)	2,3,6,7,8

Justification

K_{oc} – Thirty six literature values were obtained. The majority of values were in the range 10 to 46.77, 9 values outside of this range (exceeding 90 ml/g) were conservatively discounted. A uniform PDF was selected.

Henry's Law Constant - Seventeen literature values were obtained. Twelve values were between 1.29×10^{-5} and 2.9×10^{-5}, other values were significantly higher relative to this range and were conservatively discounted. Based on the distribution of the 12 values, a uniform PDF was selected.

Half Life in Groundwater - Based on the most conservative range of half lives for anaerobic biodegradation in water, a uniform PDF with a range 8 to 20 days was selected.

Solubility – Literature values for solubility ranged between 82,800 and 91,000 mg/l with no clear distribution. A uniform PDF was therefore selected.

Simazine – CAS 122-34-9

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular (39.81,140,421.70)	1
Henry's Law Constant (dimensionless)	Loguniform (1.37e-8,1.37e-7)	1,3
Half Life (days) in groundwater	Uniform(75,174)	1
Maximum Solubility (mg/l)	Uniform(3.5,7.4)	1,3

Justification

K_{oc} – Forty six values were obtained with the majority of values between 39.81 and 421.7 ml/g. Five values that significantly exceeded this range were conservatively discounted. Based on the histogram of the remaining values, a midpoint of 140 was selected.

Henry's Law Constant – Six values were obtained one of which (3.39×10^{-6}) was significantly higher relative to the other values and therefore conservatively discounted. Given that there was one order of magnitude between the maximum and minimum of the remaining values with no clear distribution, a loguniform PDF was selected.

Half Life in Groundwater - Based on the most conservative available values for half life in groundwater a uniform PDF was selected.

Solubility – Fourteen solubility values were selected generally in the range 3.5 to 7.4 mg/l. A uniform PDF with this range was selected discounting one higher value of 15.1 mg/l.

Toluene – CAS 108-88-3

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular (38.9,160,269.15)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Triangular (0.193,0.266,0.273)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform(110,210)	1
Maximum Solubility (mg/l)	Uniform(526,590)	2,3,6,7,8

Justification

K_{oc} – Thirty five literature values were obtained. Of these, four values exceeding 500 ml/g were conservatively as they were significantly higher than the other values and did not fit the PDF. Based on the histogram of the remaining data, a triangular distribution was selected with a midpoint of 160.

Henry's Law Constant – A triangular PDF was selected based on 31 literature values and the histogram of the values. Two values were excluded from the PDF as they were significantly higher than the other values. A midpoint of 0.266 was selected (the Environment Agency recommended value – Reference 2) based on the histogram.

Half Life in Groundwater - The most conservative half lives from literature values were selected with a uniform PDF.

Solubility – There was no clear distribution in the range of solubility values and therefore a uniform PDF was selected.

Xylenes – CAS 1330-20-7

Property	Distribution & Input	Data Source
K_{oc} (ml/g)	Triangular (74,250,616.59)	1,2,6,7,8
Henry's Law Constant (dimensionless)	Triangular (0.12,0.25,0.636)	1,2,3,6,7,8
Half Life (days) in groundwater	Uniform(112,360)	1
Maximum Solubility (mg/l)80	Uniform(161,200)	2,3,6,7,8

Justification

K_{oc} – Thirty eight literature values were obtained. Thirty six values were in the range 74 to 616.59, with two values significantly higher which were conservatively discounted. Based on the histogram of the data, a triangular PDF was selected with a midpoint of 250.

Henry's Law Constant – Thirty six values were obtained between 0.12 and 0.636. Based on the histogram of the data, a triangular PDF was selected with a midpoint of 0.25.

Half Life in Groundwater - The most conservative values of anaerobic half life in water and groundwater were selected with a uniform PDF.

Solubility - There was no clear distribution in solubility values. One value 106 mg/l was much lower than all other values and therefore conservatively discounted, a uniform PDF was selected for the remaining values.

APPENDIX G

CONTAMINANTS OF CONCERN – LITERATURE VALUES

4-chloro-2-methylphenol Koc Literature Values

Reference	Log Koc	Koc (ml/g)
5		124
5		645
11		0.22
11		400
11		14
11		700

Value greater than selected range of values

Value lower than selected range of values

4-chloro-2-methylphenol Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
Unit			
3	1.30E-06		5.31E-05
5	1.00E-06		4.09E-05
11		0.11	4.44E-05
11		1.65	6.66E-04

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

Value lower than selected range of values

4-chloro-2-methylphenol Biodegredation Groundwater Half Life Literature Values

Reference	Minimum	Maximum	(days)
No data available			

4-chloro-2-methylphenol Maximum Solubility Literature Values

Reference	Solubility (mg/l)
3	4000
5	4000
11	2300

1,2-Dichloroethane Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	1.28	19.05461
1	1.51	32.35937
1	1.06	11.48154
1	1.19	15.48817
1	1.48	30.19952
1	2.18	151.3561
1	1.15	14.12538
1	1.09	12.30269
1	1.34	21.87762
1	1.7	50.11872
1	1.64	43.65158
2	1.3	43.65158
6		28
7		76
7		22
7		34
8		19.6

Value greater than selected range of values

Value lower than selected range of values

1,2-Dichloroethane Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
Unit			
1		99	0.039937
1		123.9	0.049981
1		111.3	0.044898
1		174	0.070192
1		110	0.044374
1		111.5	0.044979
1		143	0.057686
1		92	0.037113
1		70.8	0.028561
1		101	0.040743
1		152	0.061317
1		182	0.073419
1		110	0.044374
1		185	0.074629
1		319	0.128685
1		122.5	0.049417
1		5.3	0.002138
1		8.99	0.003627
1		102.1	0.041187
1		110	0.044374
1		95.8	0.038646
1		185.2	0.07471
1		102	0.041147
1		133.1	0.053693
1		92.3	0.037234
2		121	0.048811
3	0.00118		0.048232
6	0.0013		0.053137
7			0.0401
8	0.00127		0.051911

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

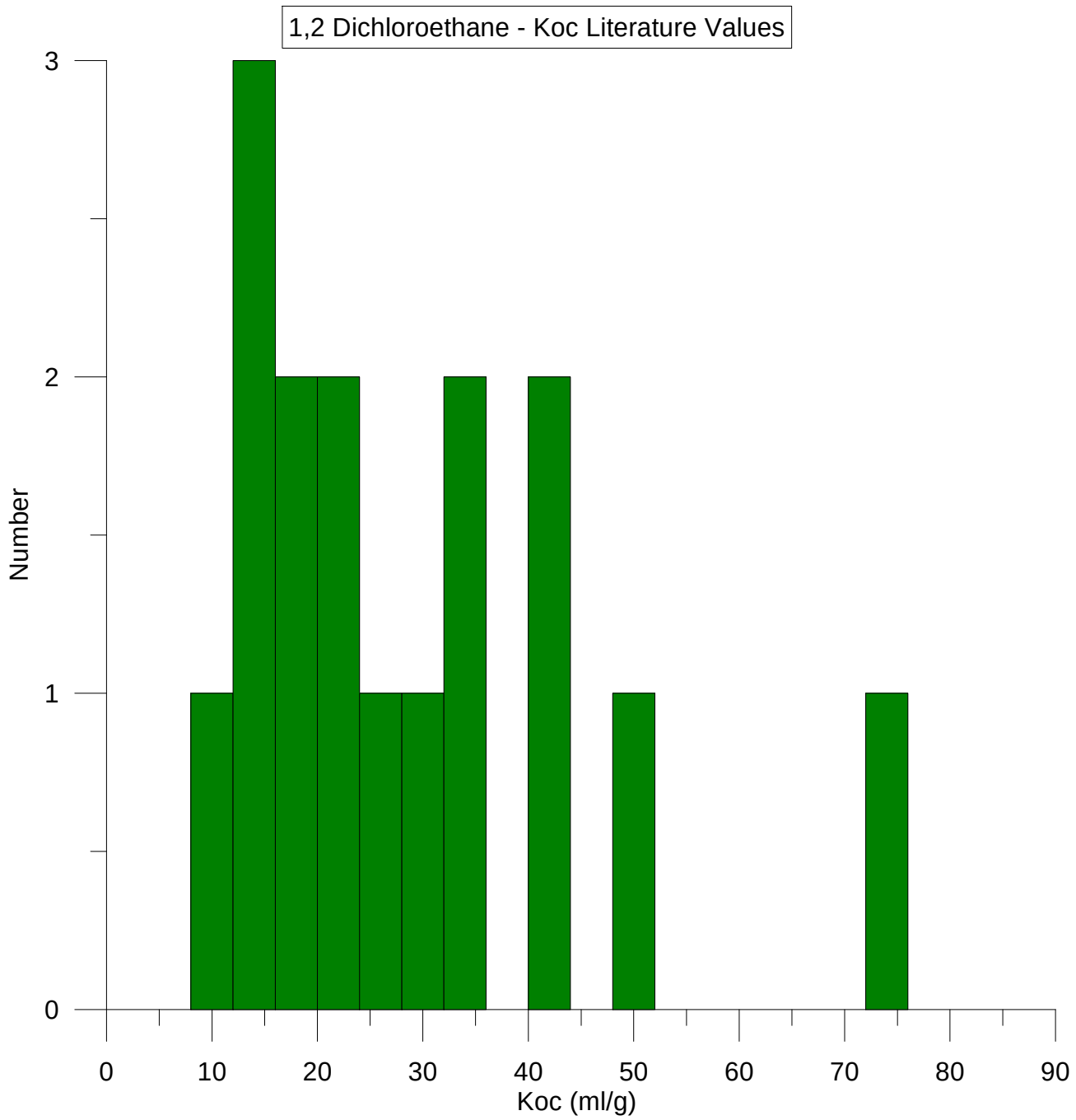
Value lower than selected range of values

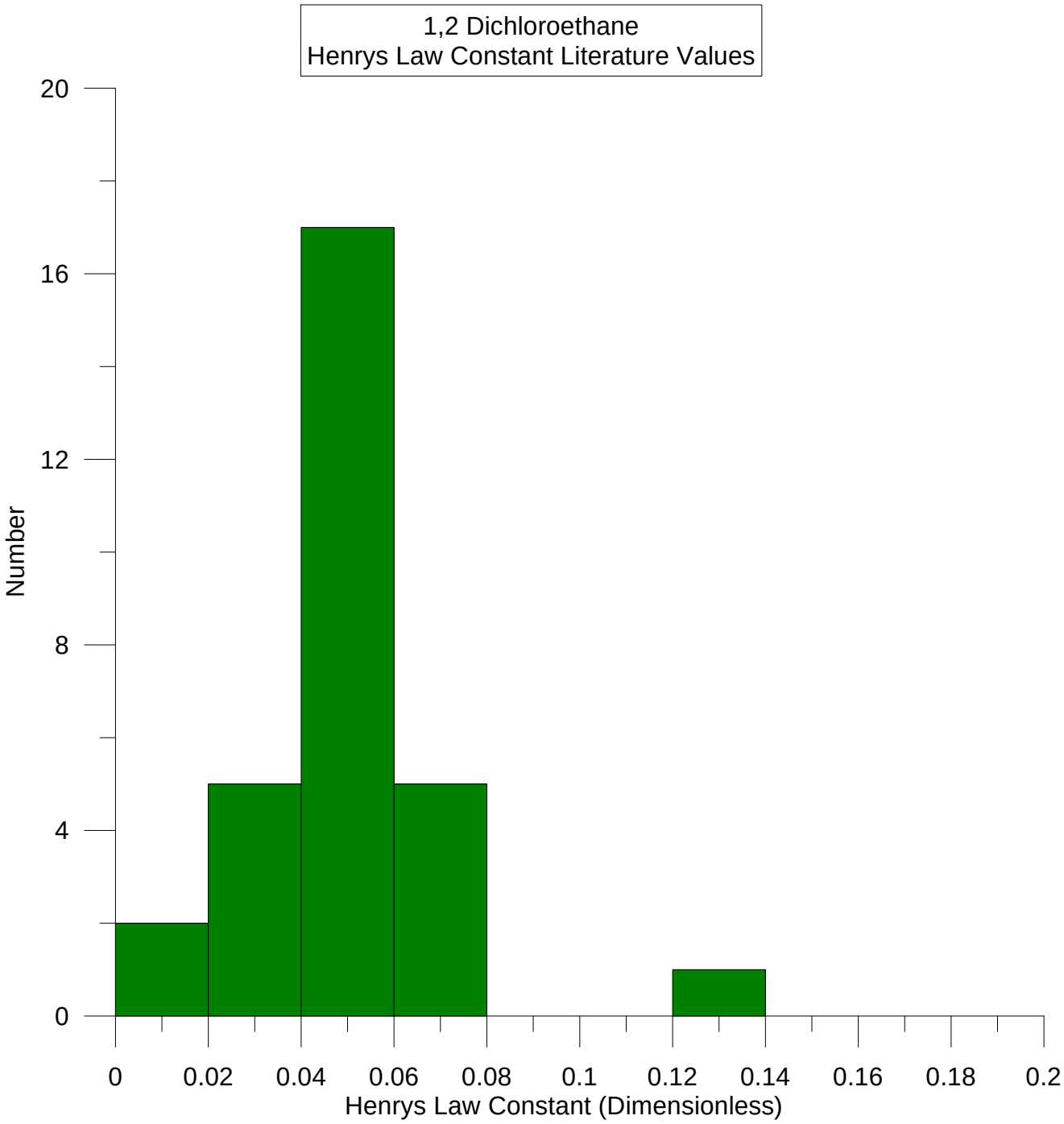
1,2-Dichloroethane Biodegredation Groundwater Half Life Literature Values

Reference	Minimum	Maximum	(days)
1	400	720	Biodegredation anaerobic half life in water
1	100	360	Aerobic half life in groundwater

1,2-Dichloroethane Maximum Solubility Literature Values

Reference	Solubility (mg/l)
2	8680
3	8600
6	8300
7	8520
8	8310


1,2 Dichloroethane - Koc Literature Values
Number
0
1
2
3
0
10
20
30
40
50
60
70
80
90
Koc (ml/g)


1,2 Dichloroethane
Henrys Law Constant Literature Values
Number
20
16
12
8
4
0
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
Henrys Law Constant (Dimensionless)

1,2 Dichlorobenzene Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	2.26	181.9701
1	3	1000
1	2.96	912.0108
1	2.62	416.8694
1	3	1000
1	4.6	39810.72
1	2.34	218.7762
1	2.59	389.0451
1	2.45	281.8383
1	3.27	1862.087
1	2.04	109.6478
1	2.43	269.1535
1	3.64	4365.158
1	3.52	3311.311
1	3.51	3235.937
1	2.45	281.8383
1	3.1	1258.925
1	2.99	977.2372
1	2.9	794.3282
1	2.62	416.8694
1	2.78	602.5596
1	2.63	426.5795
1	2.36	229.0868
1	2.48	301.9952
1	2.36	229.0868
1	2.61	407.3803
1	2.37	234.4229
1	2.51	323.5937
1	2.48	301.9952
1	2.76	575.4399
1	2.39	245.4709
1	2.4	251.1886
1	4.43	26915.35
1	3.69	4897.788
1	2.95	891.2509
1	2.5	316.2278
1	2.5	316.2278
1	2.47	295.1209
1	2.7	501.1872
1	2.69	489.7788
1	2.71	512.8614
2	2.84	691.831
6		2430
7	2.578639	379
8		379

Value greater than selected range of values

Value lower than selected range of values

0

1,2 Dichlorobenzene Henry's Law Consant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
Unit			
1		248	0.100043
1		375	0.151275
1		193	0.077856
1		122	0.049215
1		197	0.07947
1		159	0.064141
1		299	0.120617
1		141	0.056879
1		195	0.078663
1		212.7	0.085803
1		133	0.053652
2		195	0.078663
3	0.00192		0.078479
6	2.10E-03		0.085836
7	1.90E-03		0.077662
8	2.11E-03		0.086245

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

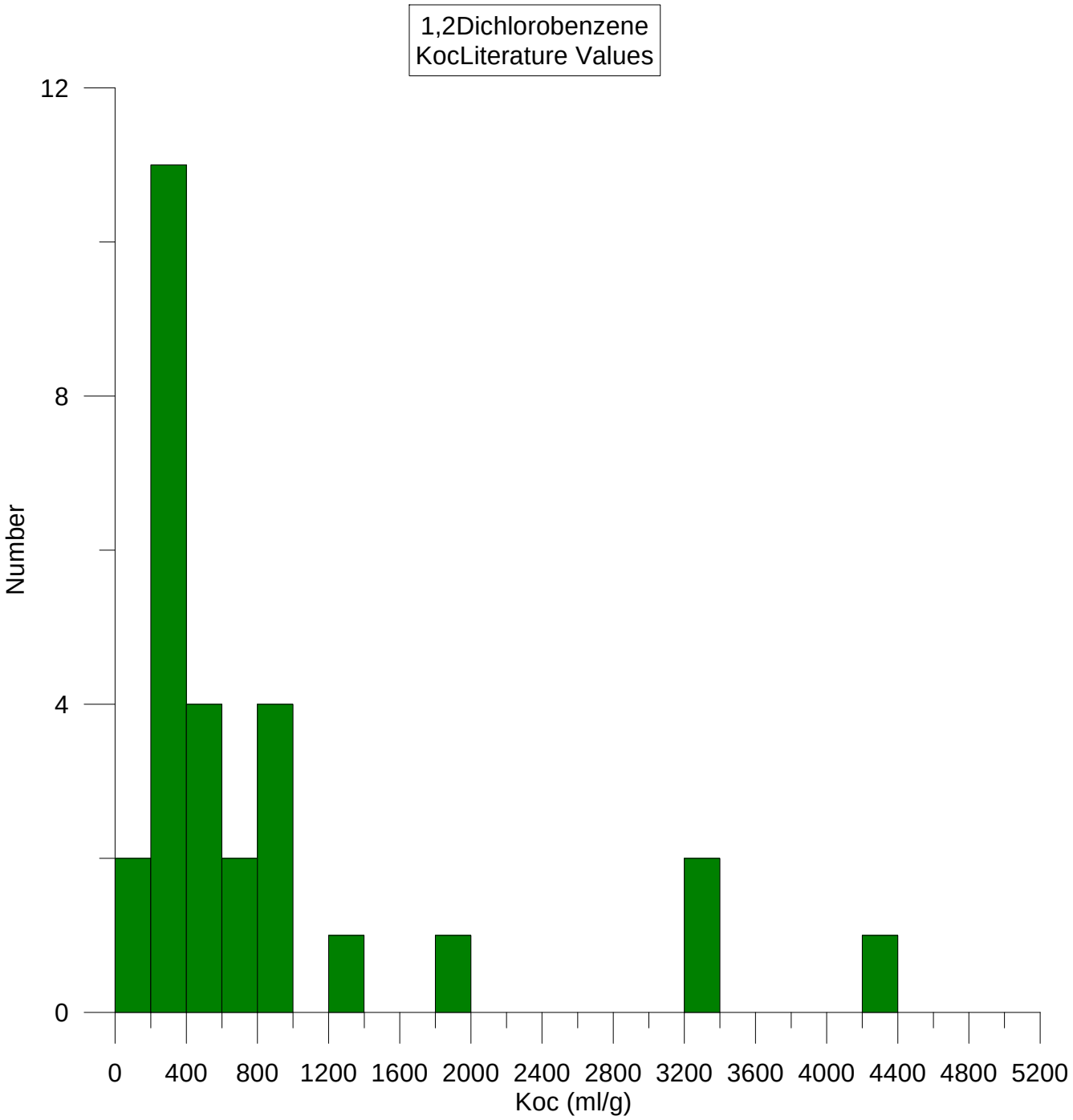
Value lower than selected range of values

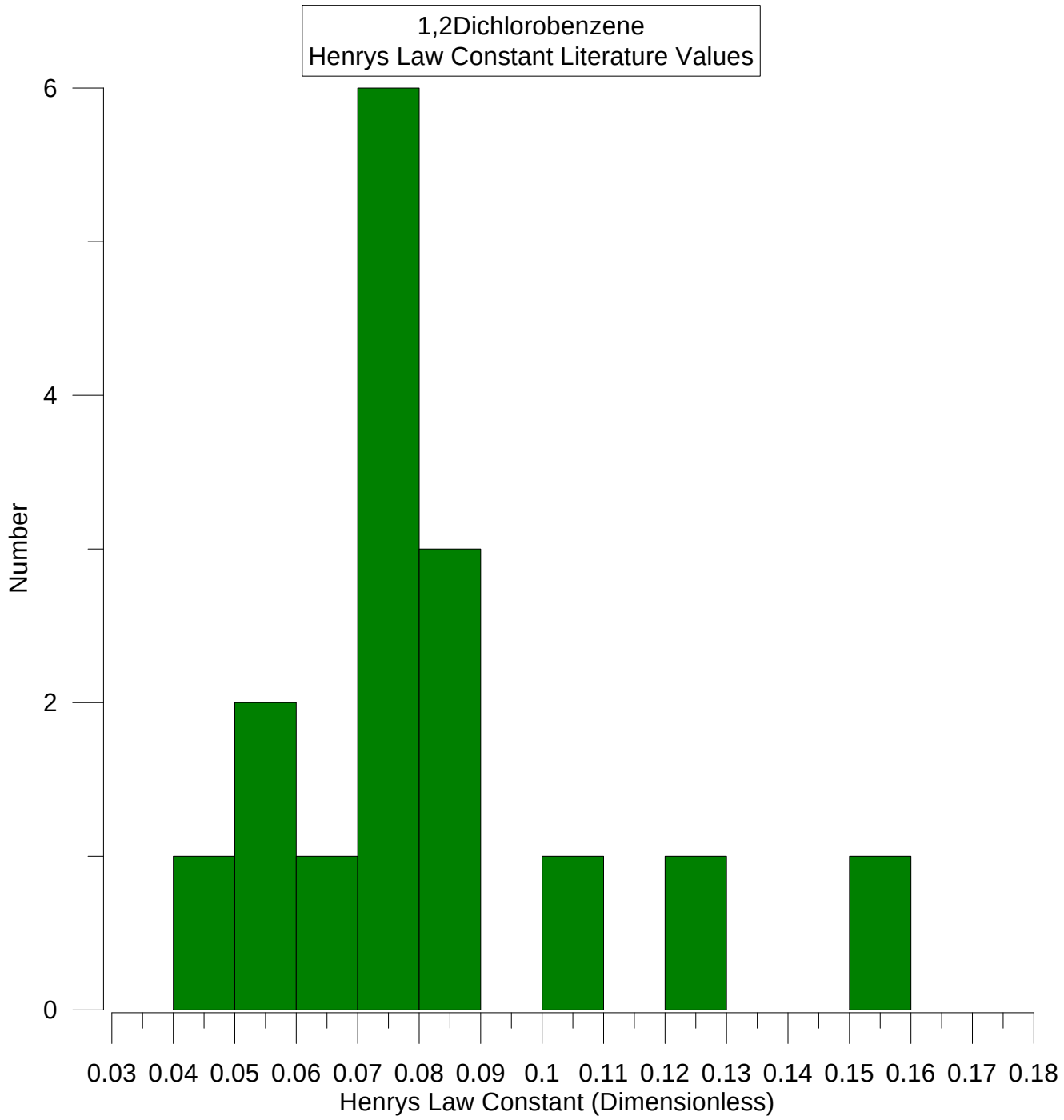
1,2 Dichlorobenzene Biodegredation Groundwater Half Life Literature Values

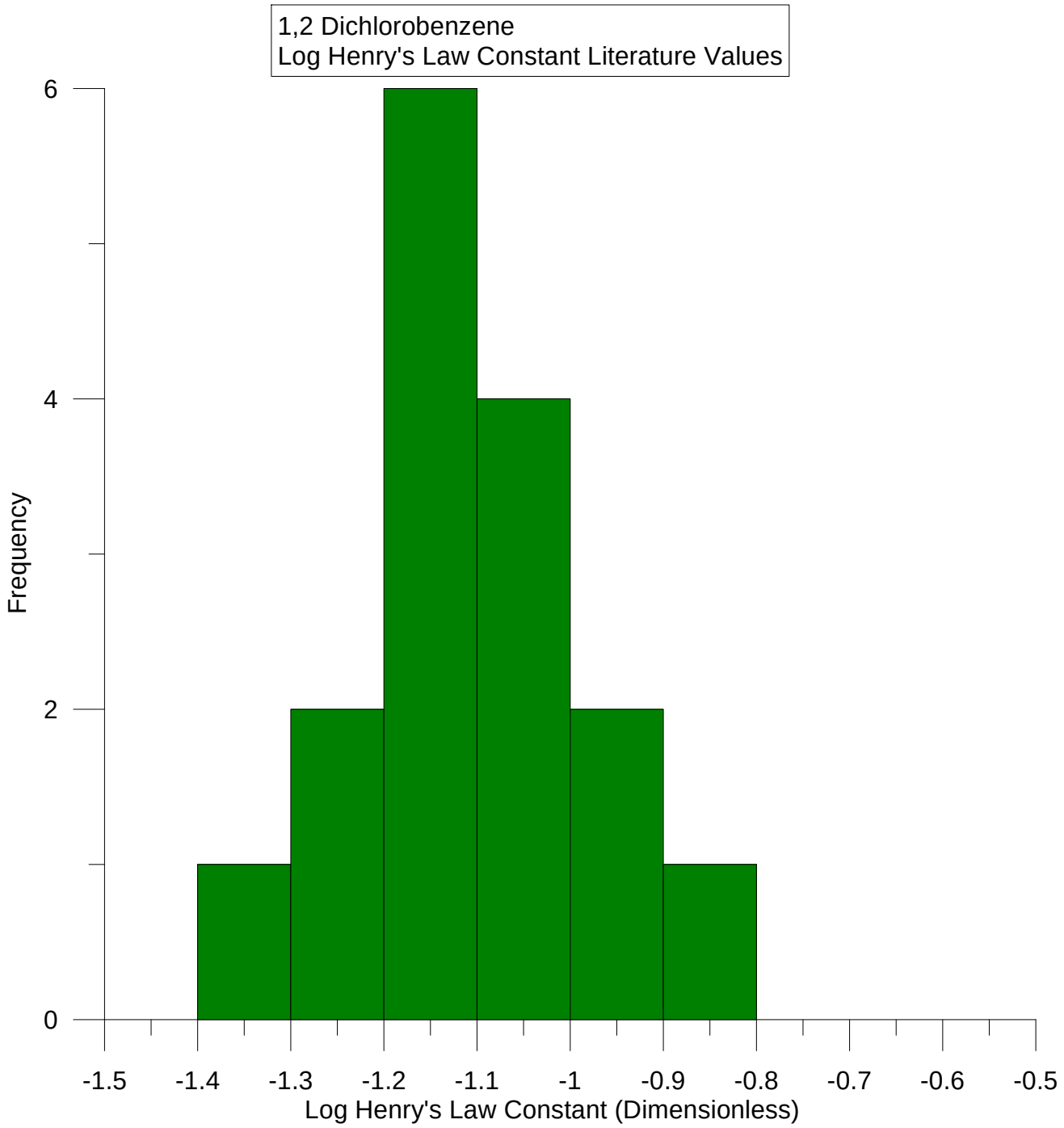
Reference	Minimum	Maximum	(days)
1	120	720	Biodegredation anaerobic half life in water
1	30	300	Based on persistence in groundwater (estimate)
1	365		Based on persistence in groundwater (estimate)
1	56	360	Observed aerobic biodegredation in groundwater

1,2 Dichlorobenzene Maximum Solubility Literature Values

Reference	Solubility (mg/l)
2	133
3	156
6	130
7	156
8	125


1,2Dichlorobenzene
KocLiterature Values
Number
12
8
4
0
0
400
800
1200
1600
2000
2400
2800
3200
3600
4000
4400
4800
5200
Koc (ml/g)


1,2Dichlorobenzene
Henrys Law Constant Literature Values
Number
0
2
4
6
0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1 0.11 0.12 0.13 0.14 0.15 0.16 0.17 0.18
Henrys Law Constant (Dimensionless)


1,2 Dichlorobenzene
Log Henry's Law Constant Literature Values
Frequency
0
2
4
6
-1.5
-1.4
-1.3
-1.2
-1.1
-1
-0.9
-0.8
-0.7
-0.6
-0.5
Log Henry's Law Constant (Dimensionless)

4,6-dinitro-o-cresol Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	2.38	239.8833
1	3.57	3715.352
1	2.44	275.4229
1	2	100
1	2.53	338.8442
1	2.41	257.0396
1	2.78	602.5596
1	3.28	1905.461
4		300
5		23
5		257

Value greater than selected range of values

Value lower than selected range of values

4,6-dinitro-o-cresol Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
Unit			
1		4.05	0.001634
1		43.22	0.017435
3	1.40E-06		5.72E-05

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

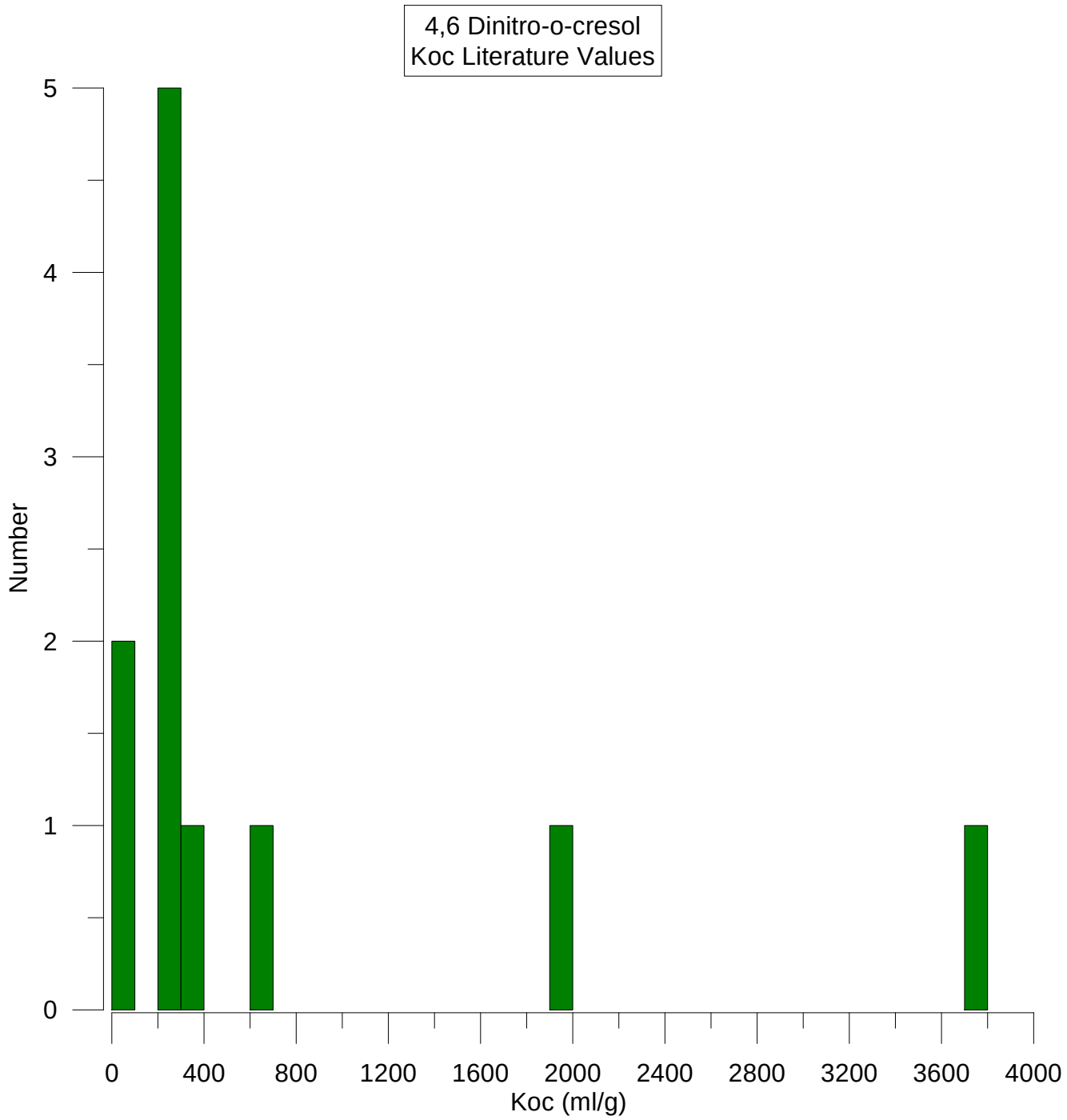
Value lower than selected range of values

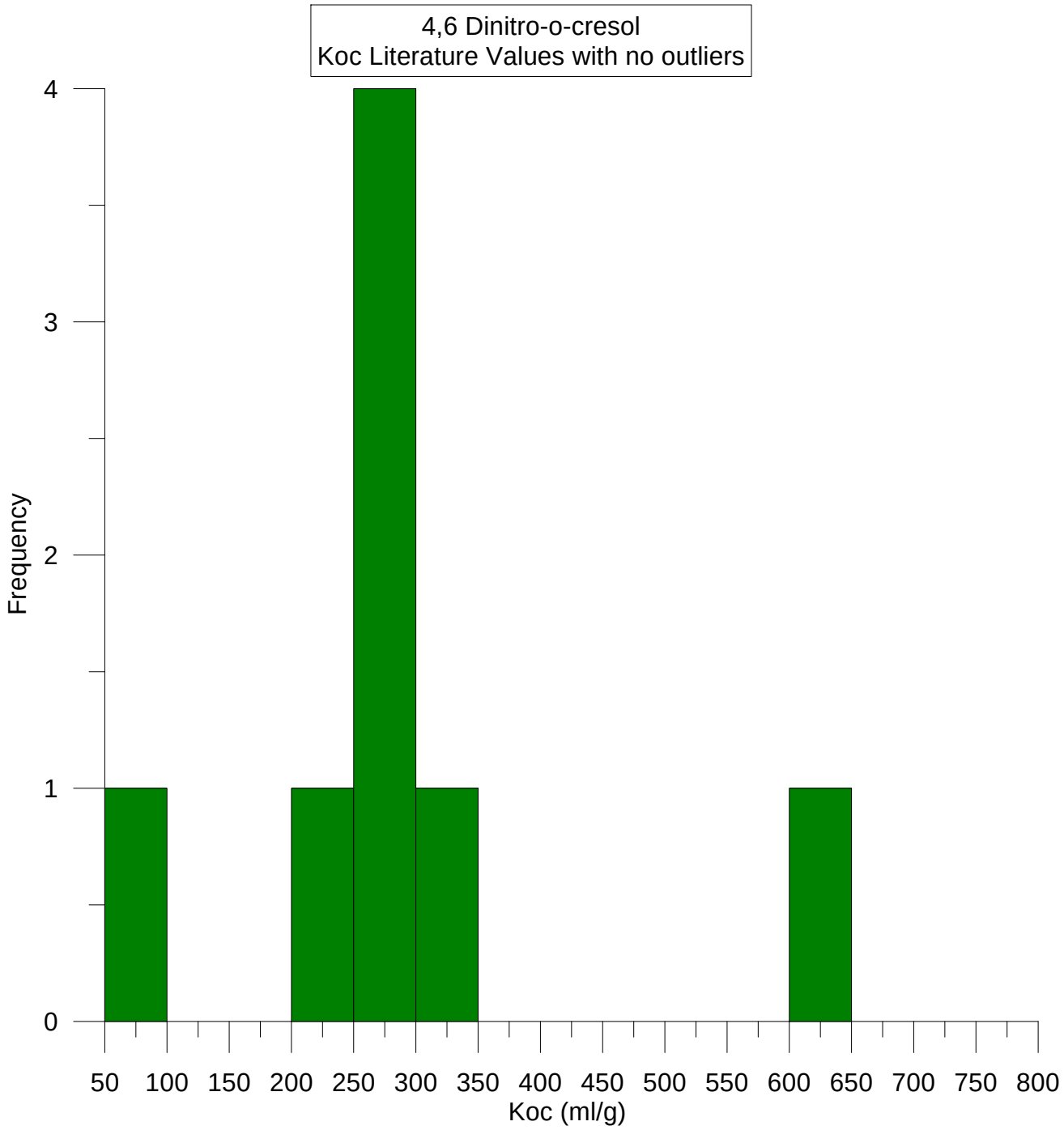
4,6-dinitro-o-cresol Biodegredation Groundwater Half Life Literature Values

Reference	Minimum	Maximum	(days)
1	2.83	42	Biodegredation in groundwater based on aerobic and anaerobic half
1	2.83	7	Biodegredation in aqueous anaerobic conditions
1	28		Biodegredation in anaerobic conditions in natural water

4,6-dinitro-o-cresol Maximum Solubility Literature Values

Reference	Solubility (mg/l)
1	258
1	250
1	290
1	198
1	150
3	198


4,6 Dinitro-o-cresol
Koc Literature Values
Number
0
1
2
3
4
5
0
400
800
1200
1600
2000
2400
2800
3200
3600
4000
Koc (ml/g)


4,6 Dinitro-o-cresol
Koc Literature Values with no outliers
Frequency
0
1
2
3
4
50
100
150
200
250
300
350
400
450
500
550
600
650
700
750
800
Koc (ml/g)

2,4,6-trichlorophenol Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	2.34	218.7762
1	3.3	1995.262
1	2.52	331.1311
1	3.84	6918.31
1	3.41	2570.396
1	2.48	301.9952
1	2.87	741.3102
1	3.02	1047.129
1	2.99	977.2372
1	3.57	3715.352
1	3.33	2137.962
1	2.75	562.3413
1	2.52	331.1311
1	3.73	5370.318
1	3.3	1995.262
1	3.34	2187.762
1	2.79	616.595
1	2.23	169.8244
1	2.79	616.595
1	3.34	2187.762
1	2.04	109.6478
1	2.5	316.2278
1	2.92	831.7638
1	3.12	1318.257
1	3.03	1071.519
1	3.02	1047.129
1	2.82	660.6934
1	3.03	1071.519
1	2.81	645.6542
1	2.25	177.8279
1	3.02	1047.129
1	3.08	1202.264
1	2.59	389.0451
1	3.03	1071.519
1	2.52	331.1311
1	2.88	758.5776
2	3.18	1513.561
6	3.633468	4300
8	2.354493	226.2

Value greater than selected range of values

Value lower than selected range of values

2,4,6-trichlorophenol Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
Unit			
1		0.405	1.63E-04
1		0.132	5.32E-05
1		0.523	2.11E-04
1		0.5687	2.29E-04
1		0.428	1.73E-04
2		9.19E-03	3.71E-06
3	2.60E-06		1.06E-04
6	4.10E-06		1.68E-04
7	7.79E-06		3.18E-04
8	4.06E-06		1.66E-04

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

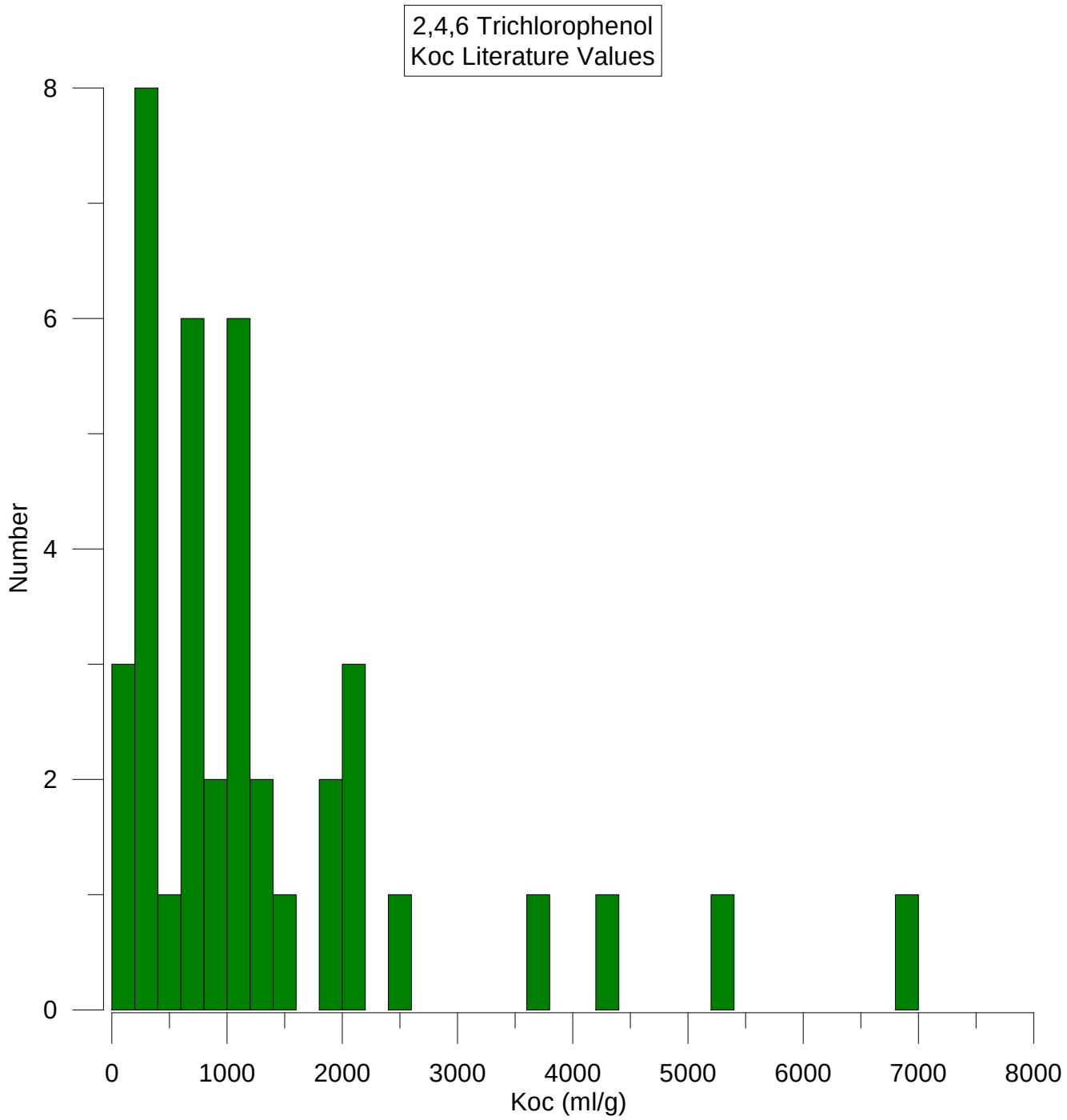
Value lower than selected range of values

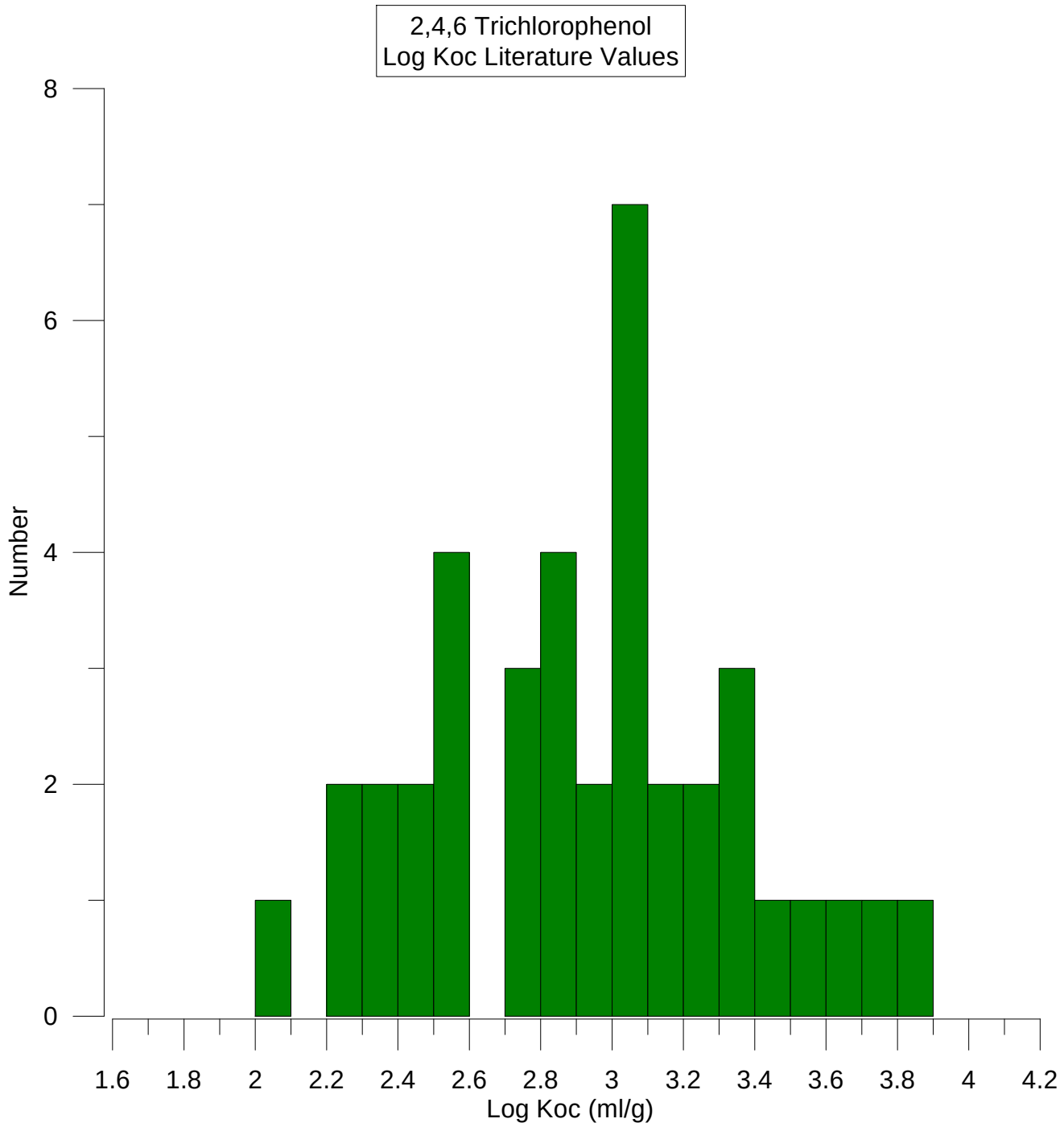
2,4,6-trichlorophenol Biodegredation Groundwater Half Life Literature Values

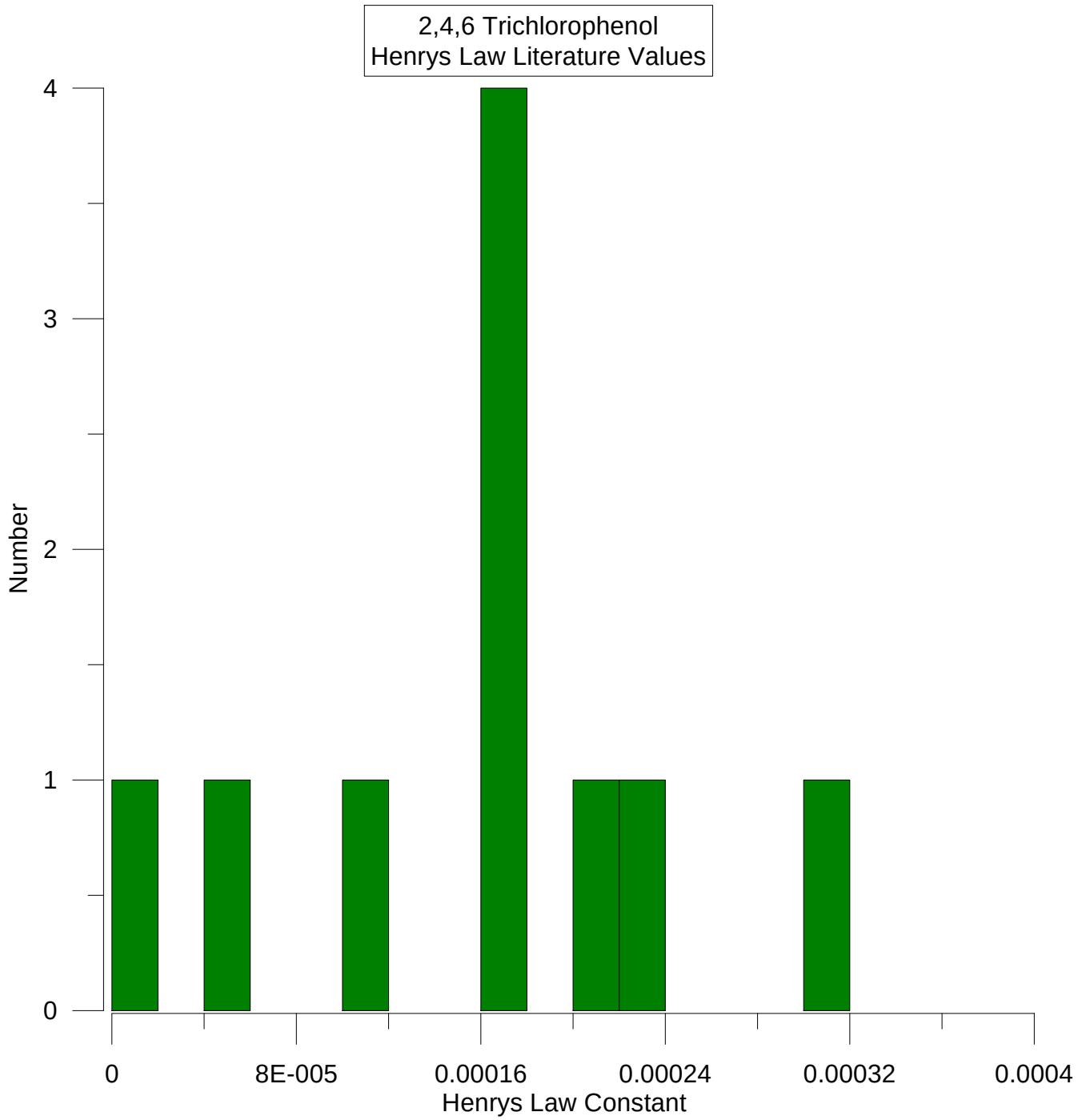
Reference	Minimum	Maximum	(days)
1	169	1820	Anaerobic aqueous half life
1	14	1820	Half life in groundwater based on aerobic and anaerobic half lives

2,4,6 trichlorophenol Maximum Solubility Literature Values

Reference	Solubility (mg/l)
2	434
3	800
6	750
7	800
8	753


2,4,6 Trichlorophenol
Koc Literature Values
Number
0
2
4
6
8
0
1000
2000
3000
4000
5000
6000
7000
8000
Koc (ml/g)


2,4,6 Trichlorophenol
Log Koc Literature Values
Number
0
2
4
6
8
1.6
1.8
2
2.2
2.4
2.6
2.8
3
3.2
3.4
3.6
3.8
4
4.2
Log Koc (ml/g)


2,4,6 Trichlorophenol
Henrys Law Literature Values
Number
4
3
2
1
0
0
8E-005
0.00016
0.00024
0.00032
0.0004
Henrys Law Constant

Bis-2(chloroehtyl)ether Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	1.38	23.98833
1	1.14	13.80384
3	1.88	75.85776
6		15
7		76
8		76

Value greater than selected range of values

Value lower than selected range of values

Bis(2-chloroehyl)ether Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
1		1.32	5.32E-04
1		28.97	1.17E-02
3	1.70E-05		6.95E-04
6	2.10E-05		8.58E-04
7			7.38E-04
8	2.13E-05		8.71E-04

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

Value lower than selected range of values

Bis (2-chloroehtyl)ether Biodegredation Groundwater Half Life Literature Values

Reference	Minimum	Maximum	(days)
1	56	360	Half life in groundwater
1	112	720	Anaerobic biodegredation in water

Bis(2-chloroehtyl)ether - Maximum Solubility Literature Values

Reference	Solubility (mg/l)
1	10200
1	10400
1	10200
3	17200
6	12000
7	17200
8	11800

Cis-1,2-dichloroethene Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	1.69	48.97788
1	1.84	69.1831
6		67
7		35.6
8		35.6

Value greater than selected range

Value lower than selected range

Cis 1,2-dichloroethene Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
1		342.2	1.38E-01
1		1970	7.95E-01
1		2370	9.56E-01
1		441.1	1.78E-01
1		460	1.86E-01
1		745.5	3.01E-01
1		324	1.31E-01
1		496	2.00E-01
1		740	2.99E-01
1		331	1.34E-01
1		518	2.09E-01
1		751	3.03E-01
1		341	1.38E-01
1		444	1.79E-01
1		413.4	1.67E-01
1		319	1.29E-01
1		674.5	2.72E-01
3	4.80E-03		1.96E-01
6			1.84E-01
7	4.08E-03		7.54E-01
8	4.51E-03		1.84E-01

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

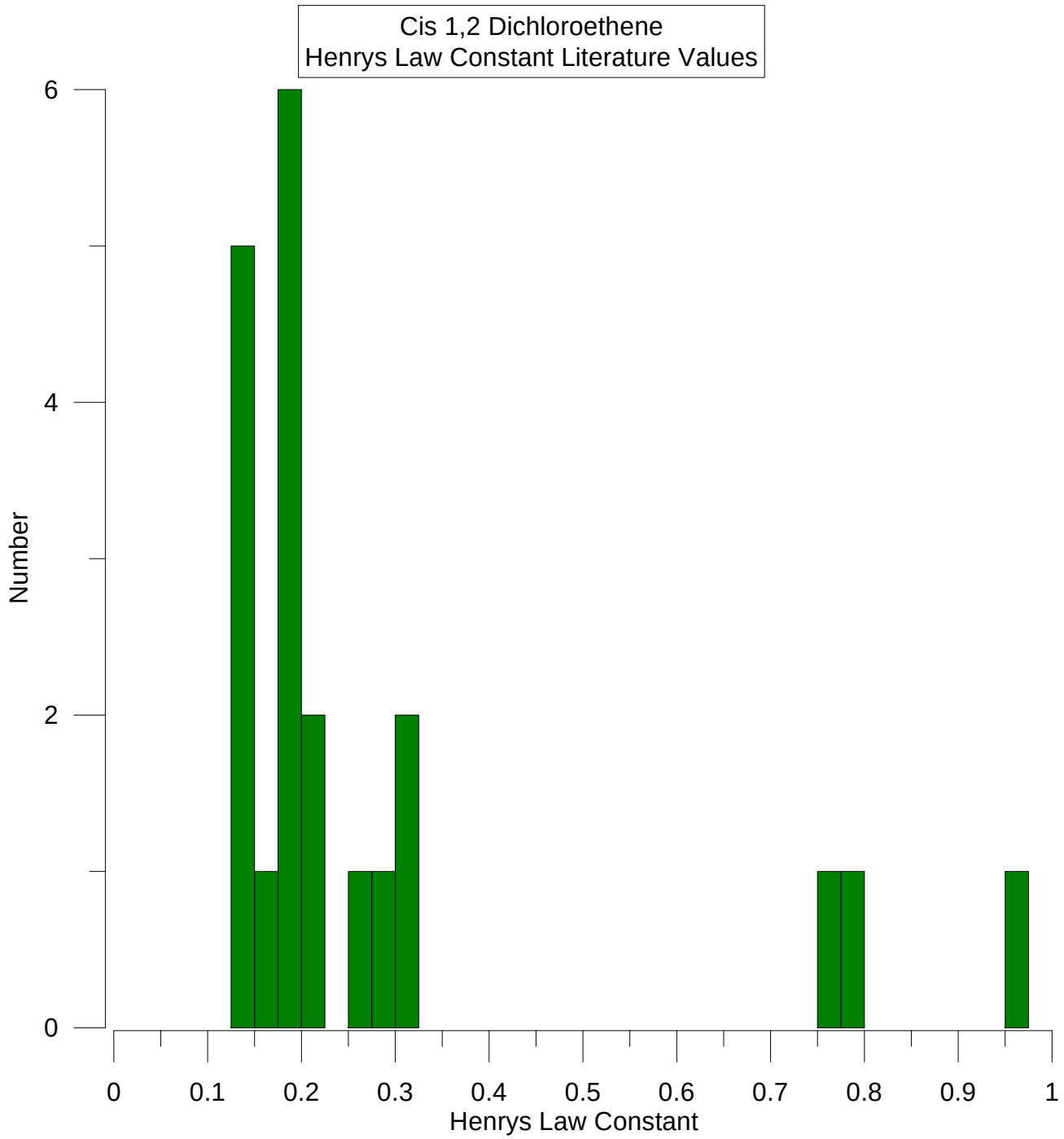
Value lower than selected range of values

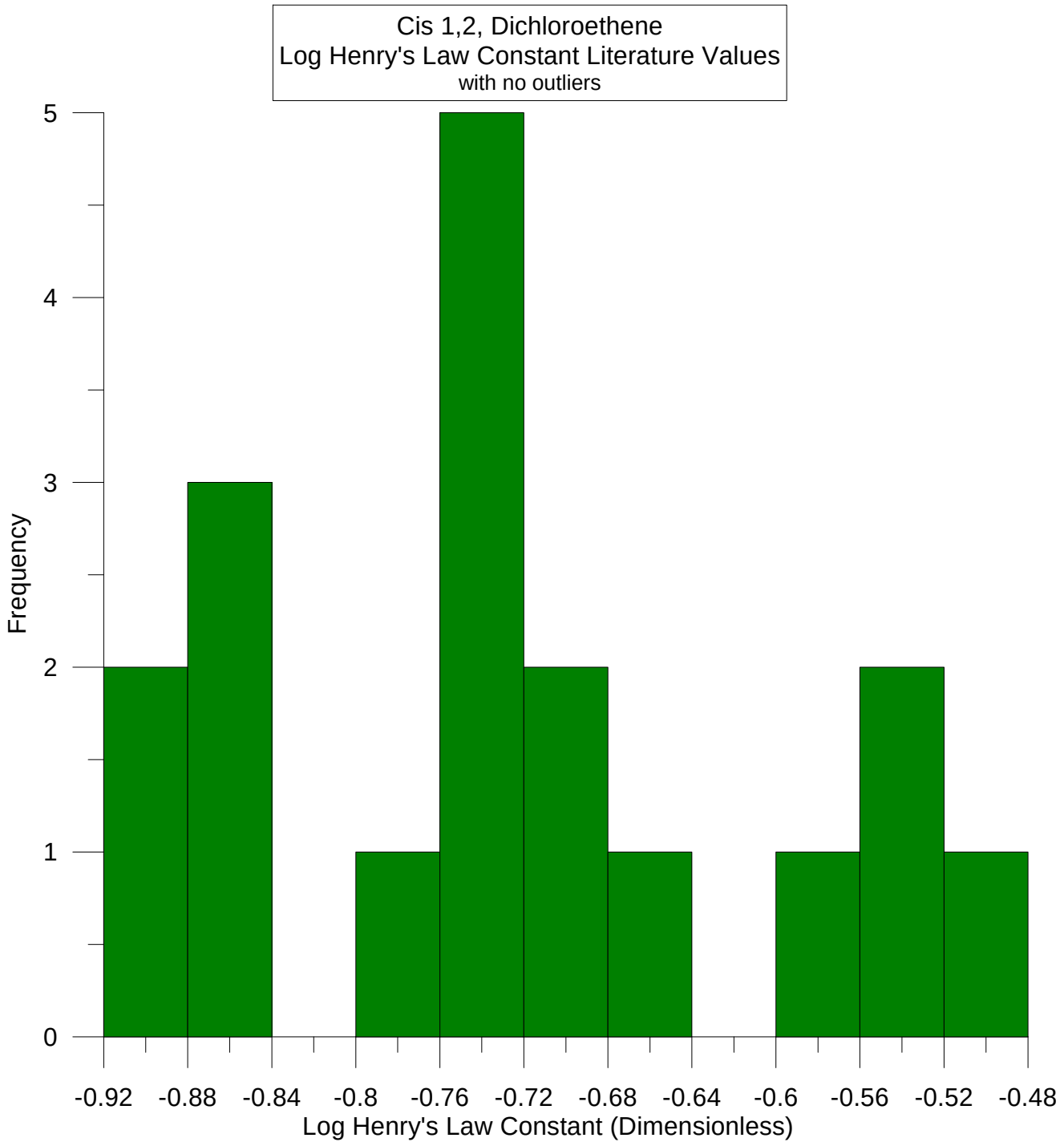
Cis-1,2-dichloroethene Biodegredation Groundwater Half Life Literature Values

Reference	Minimum	Maximum	(days)
1	112	720	Anaerobic biodegredation in water
1	56	2875	Environmental half life in groundwater (aerobic)

Cis-1,2-Dichloroethene Maximum Solubility Literature Values

Reference	Solubility (mg/l)
1	6410
3	6410
6	4900
7	4900
8	4910


Cis 1,2 Dichloroethene
Henrys Law Constant Literature Values
Number
0
2
4
6
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Henrys Law Constant


Cis 1,2, Dichloroethene
Log Henry's Law Constant Literature Values
with no outliers
Frequency
0
1
2
3
4
5
-0.92
-0.88
-0.84
-0.8
-0.76
-0.72
-0.68
-0.64
-0.6
-0.56
-0.52
-0.48
Log Henry's Law Constant (Dimensionless)

Cyclohexanone Koc Literature Values

Reference	Log Koc	Koc (ml/g)
1	1	10
5		15
10	1.823	66.52732

Value greater than selected range

Value lower than selected range

Cyclohexanone Henry's Law Constant Literature Values

Reference	atm.m3/mol	Pa.m3/mol	Unitless
1		1.216	4.91E-04
1		2.266	9.14E-04
1		5.179	2.09E-03
3	9.00E-06		3.68E-04
5	9.00E-06		3.68E-04
10	1.25E-05		5.11E-04

Conversion Factors	
atm.m3/mol to unitless	40.87451
PA.m3/mol to unitless	0.000403

Value greater than selected range of values

Value lower than selected range of values