Water Resources Research

Supporting Information for

Hydrophobic organic contaminant transport property heterogeneity in the Borden Aquifer

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Additional Supporting Information (Files uploaded separately)

Captions and headings for Tables S2 and S3

Introduction

The Supporting Information includes the complete data set of k, K_d, and indicator data, as described within the manuscript. The indicator data are Table S2. The k and K_d results are in Table S3. The lithofacies codes used in prior published manuscripts and herein are compared in Table S1. The various other files provide information on summary statistics, sources of uncertainty from field and laboratory procedures, and provide quantitation of the uncertainties where possible. Data from the new cores and cores from the original study as reported in Divine [2002] are differentiated.

Text S1. Core collection method detail.

Variable core spacing was used to facilitate development and testing of statistical models to describe horizontal heterogeneity while managing the time required for detailed data collection. The core spacing was different in each of the three approximately 10 m horizontal sections: 0.5 m in the south section (cores 5.0 to 15.0 N), 0.25 m in the central section (cores 15.5 to 25.25N) and 1 m in the north section (cores 25.5 to 35.5N) (Figure 3). The 0.5 m was selected for the south section in order to insure that caving at prior core removal locations did not affect the new cores. The 0.25 was selected as the finest reasonable spacing as the transect was extended into the central section. A 1 m spacing was used in north section to expand transect as far as possible within the time constraints imposed by the laboratory analyses. Although most cores were collected along the previously established transect, some cores were taken approximately 25 cm 'off' the main transect line for practical reasons, e.g. the core barrel was refused at a shallow depth preventing core collection at the targeted location. The core collection method was the same as in our prior work at Borden [*Allen-King et al.*, 1998; *Allen-King et al.*, 2006] in which cores are collected without a drill rig in 5 cm diameter aluminum tubing following the method of Starr and Ingleton [1992] . In order to improve vertical control (compared to surveying ground surface), we established temporary survey benchmarks at approximately 1 m intervals and reference core elevation to these benchmarks. The relative elevations of the temporary markers were surveyed to permanent markers previously established within the sandpit area at CFB Borden (approximately 6 cm elevation discrepancy between the current and prior core sets). Despite these additional steps, comparisons between neighboring cores showed offset that was corrected by minor (cm) adjustment based on aligning a reference bounding surface. In order to improve the consistency with which we viewed the sediment both between core locations and within cores, a new measure in this study was to record core rotation during extraction and to note and account for alignment at all junctures of core cutting.

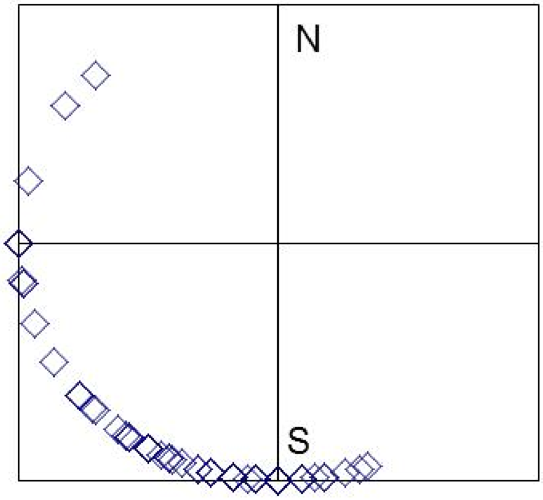


Figure S1. Relative core rotation at retrieval for cores collected for this study. 60% of cores were oriented within ± 22.5 degrees of the median and 84% were within ± 45 degrees of the median.

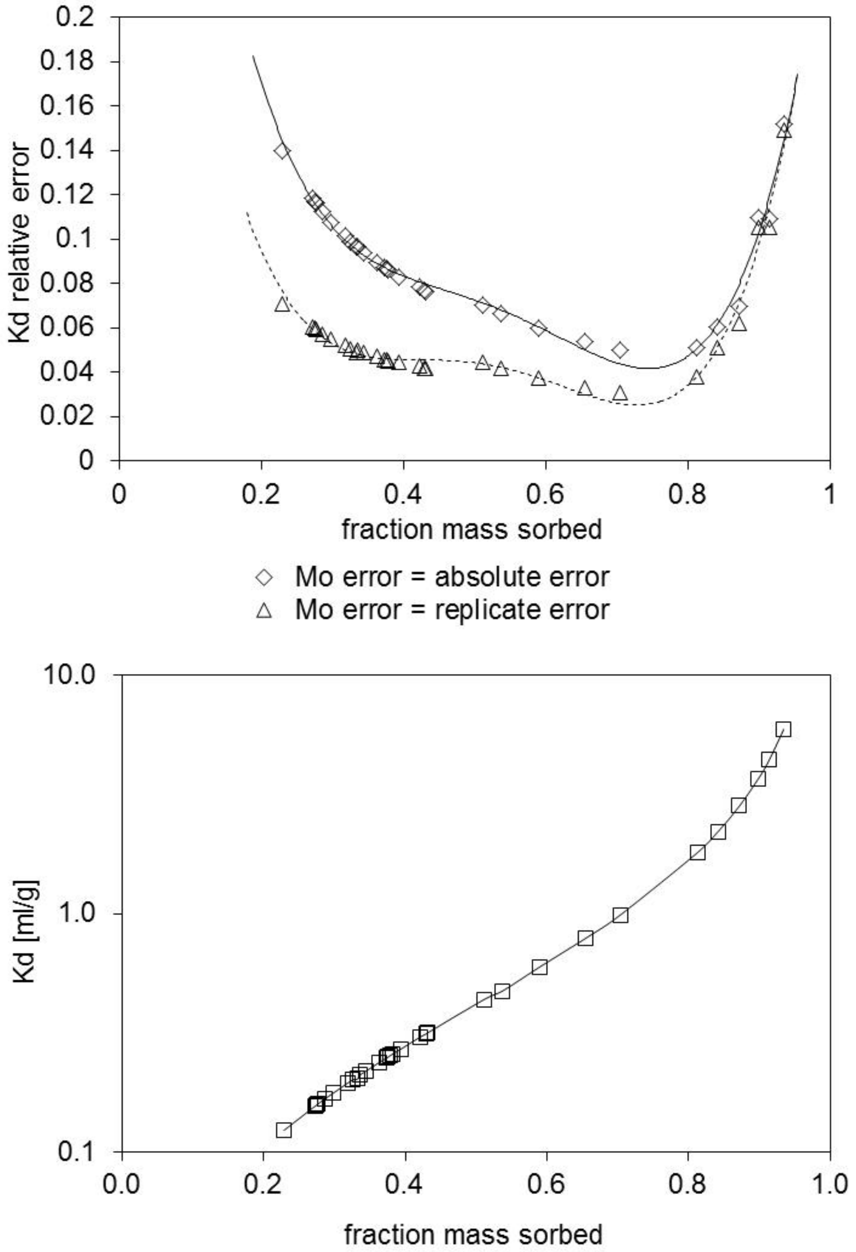


Figure S2. The relative error in K_d (ε) (a) and K_d (b) as functions of the fraction of PCE sorbed for one experiment set. The ε_{Kd} is determined by standard error propagation techniques, as described in *Allen-King et al.* [2006]. The relative errors are less than 15% for most samples, and depend upon the presumed Mo error, as described in *Ball and Roberts* [1991]. Relative error increases slowly with declining sorbed mass fraction as the difference between the initial and aqueous plus gas phase masses become comparable. Relative error at the high end of the range increases more sharply when the equilibrium aqueous concentration is substantially below the lowest calibration point. Relatively few of the total samples fell into the latter category. Most of these high sorbing samples were reanalyzed in a 5 mL ampoule system with lower sediment mass fraction, and consequent equilibrium sorbed PCE mass fraction, and the data retained in the reported data set reflects the latter value.

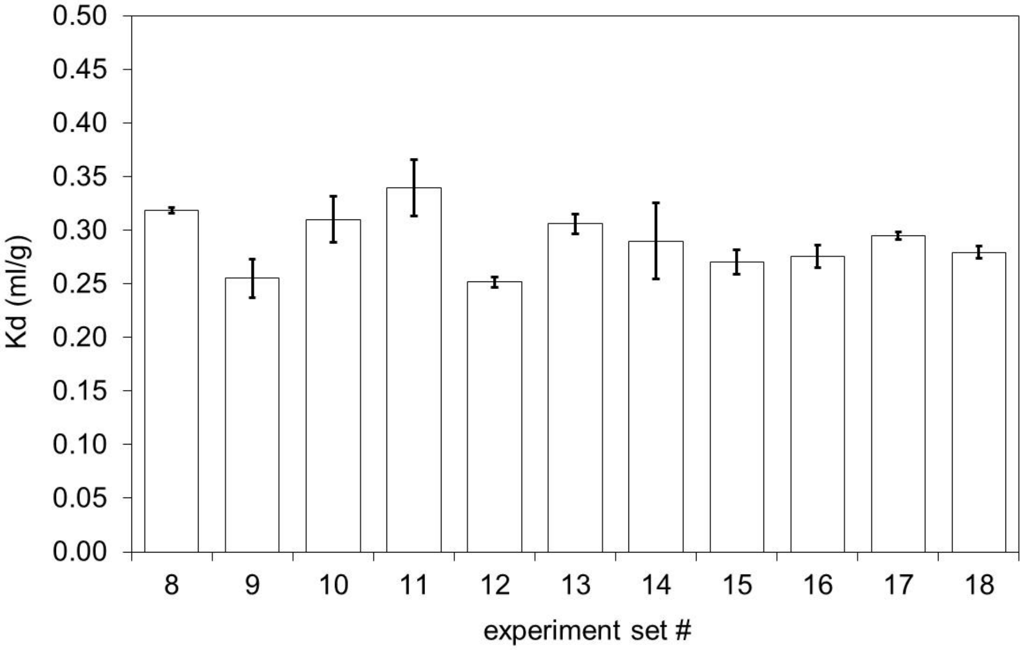
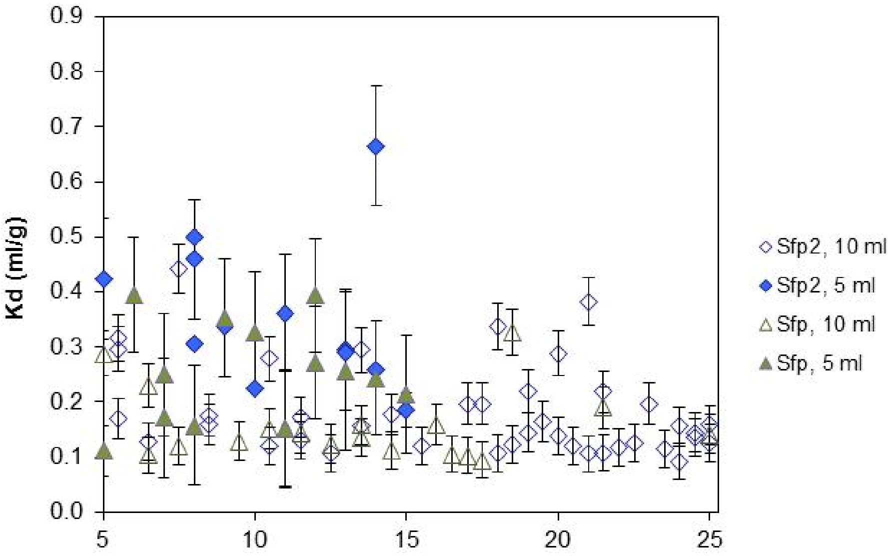


Figure S3. Triplicate bulk Borden (reference) sample measurements for 11 experiment sets completed in 10 ml ampoules. The error bars indicate + 1σ.These reference sample measurements indicate the impact of cumulative analytical errors on K_d between experiment sets. The set-to-set coefficient of variation (CV) of 9% is comparable to the approximately 8% relative K_d error estimated by error propagation (Fig. S2) corresponding to the average K_d (=0.29 mL g-1) observed for the bulk Borden reference sample. The average CV of all sets was 5% with range of 1%-12%. The bulk (reference) sample was not analyzed in sets 1-7or 19.1. Error propagation suggests that errors in sets 2-7 and 19.1 were comparable to that shown for sets 8-18. Sets 1 and 19.5 were completed in 5 ml ampoules. Other analytical measures indicate that the analytical uncertainties in set 1, the initial experiment set, were larger than the errors measured in sets 2-19. Comparison of the mean value for the 5 ml ampoule measurements of the reference sample in experiment 19.5 suggests that these measurements and those in experiment set 1may exhibit a slight bias towards high values for an unexplained reason. Samples measured in 5 ml ampoules in experiment 19 were completed because either 1) the very high K_d values for these samples caused the aqueous solution concentration to be substantially below the lowest calibration standard in a prior measurement, or 2) the sample needed to re-measured (e.g. replaced due to breakage of the original vial) and too little sample remained to complete a quality measurement in a 10 ml vial.



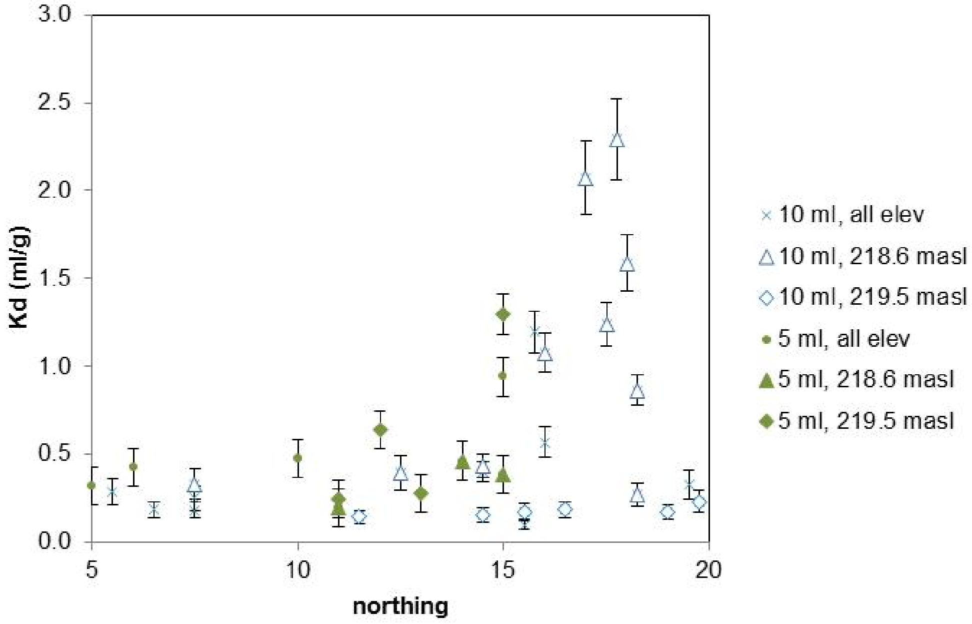
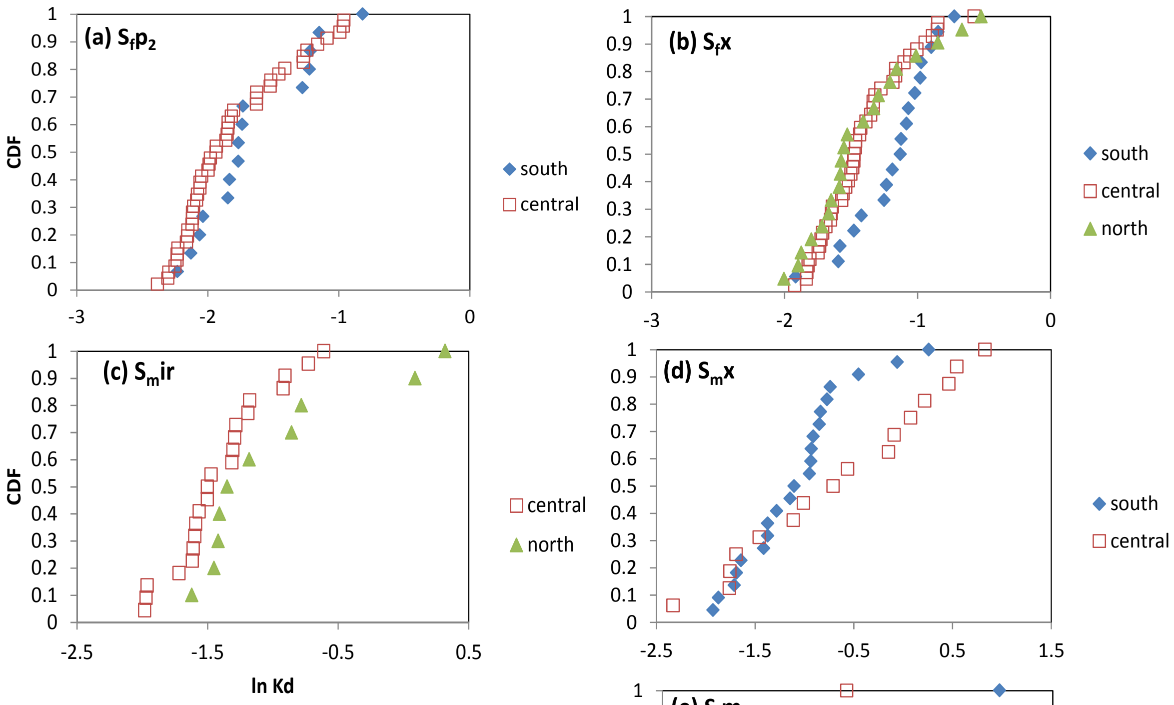


Figure S4a. Significant differences in ln K_d were observed for the S_fp and S_fp_2 samples, the units with the lowest ln K_d values. The method used in the current work (designated 10 ml) produced lower values compared to the original method (designated 5 ml). These differences are ascribed to analytical error. The error bars indicate $\pm 2\varepsilon_{Kd}$.

Figure S4b. The ln K_d of the S_mx unit (including samples from the S_mx_3 and S_mx_2) plotted for samples measured in the current study and in the original study for cores numbered 5 through 20. The apparent difference between measurements in the original and current study in cores numbered 5-15 is attributable to high variability within this unit and small sample numbers. The error bars indicate $\pm 2\varepsilon_{Kd}$. Analytical uncertainties for all but the lowest K_d sample range are comparable for the two studies. (Note the vertical scale difference between Figures S4a and S4b.)



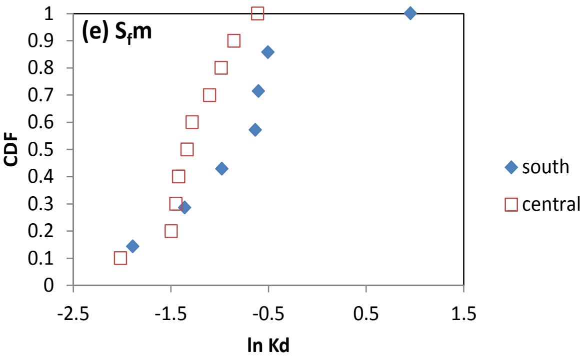


Figure S5. The CDF for ln K_d for the units that exhibited differences by section at a potentially significant level (0.05<p<0.11): (a) S_fp_2; (b) S_fx, (c) S_mir, (d) S_mx , and (e) S_fm The difference in the S_fp_2 is subtle (the ln-averages translate to 0.19 ml/g and 0.17 ml/g for the south and central sections, respectively) and ascribed to the lower than planned sample density in the south section because of subsequently discovered analytical bias. The ln K_d CDFs of the S_mir unit by section are similar, but exhibit a relatively modest 'offset' of approximately 0.2 ln K_d units near the median value, with greater differences caused by just a few very low or very high representatives out of a relatively small sample number, particularly in the northern section.

The ln K_d of the S_mx unit exhibits high variance. The CDFs of the two sections are similar for values less than the median, and differ between the 50th to 90th percentiles. The high within unit variance suggests the likelihood that neither of the two sections alone adequately sampled this unit. Hence, for the S_mx unit, sampling location and density may be responsible for the apparent differences between sections. This unit underscores the importance of identifying, or in hindsight evaluating, the extent to which the sampling strategy provides representative results.

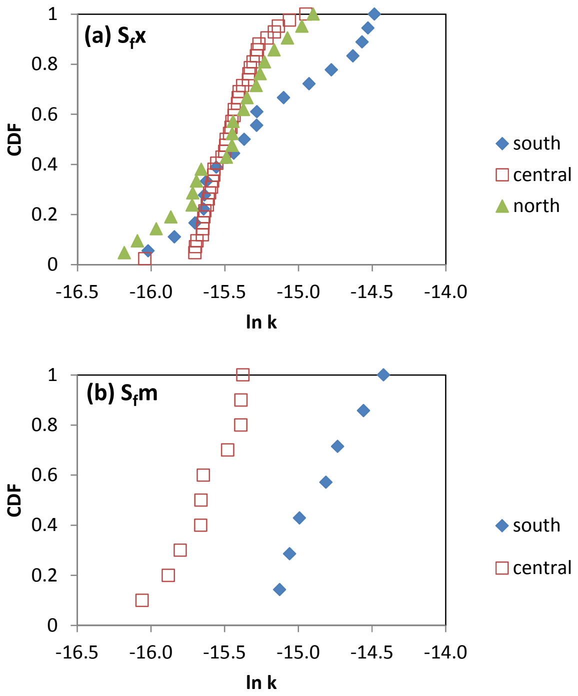


Figure S6. The CDF for ln k for the units that exhibited significant differences by section ($p<0.05$): (a) $S_f x$ and (b) $S_f m$.

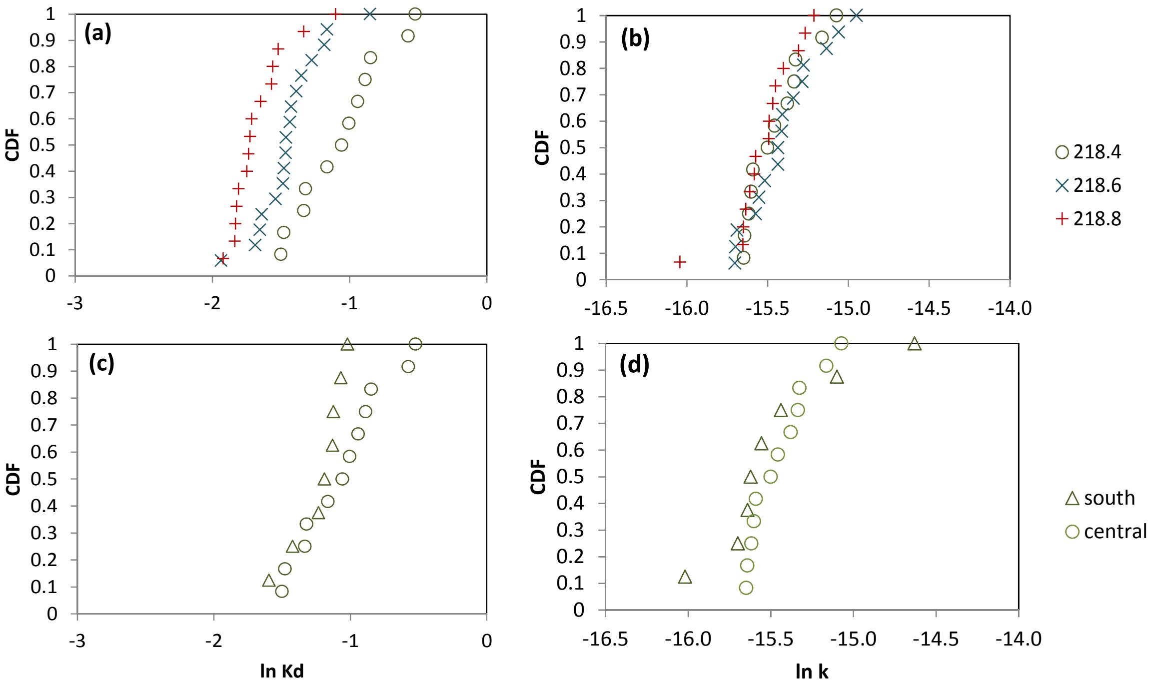


Figure S7. The S_fx CDF with contrasting elevations in the central section for ln K_d (a) and ln k (b) and contrasting sections at a consistent elevation (218.4 MASL) for ln K_d (c) and ln k (d). There is little difference between the north and central section CDFs of either property for the S_fx unit, but the south section exhibited ostensibly greater mean for both properties and greater ln k variance (Figs. S5 and S6). Most of the S_fx samples are drawn from the three lowest elevations. We find that the ln K_d of the S_fx unit exhibits a subtle but significant decrease with greater elevation in the central section, where the unit is prominent and densely sampled (Fig. S7a; -1.1, -1.4 and -1.7 for the 218.4, 218.6 and 218.8 MASL elevation samples, respectively, ANOVA p=0.011). The S_fx unit is mostly absent at 218.8 MASL in the south section because the unit was apparently eroded and replaced by a scour feature. Therefore the S_fx unit in the south section is represented primarily by samples from the lower two elevations. Contrasting samples taken from a single elevation (218.4 MASL) in the south and central sections affirms that samples taken from a similar elevation are not different (ANOVA, p= 0.199) (Fig. S7c). Therefore, we conclude that the apparent section related bias for this unit is attributable to sample distribution within the section. For the ln K_d, these findings underscore the already well known importance of sampling throughout unit thickness in order to insure representative results.

The ln *k* analysis shows no significant difference either by elevation within the central section (p=0.290) or by section at a single elevation (p=0.899) (Figs. S7b and S7d). No patterns were identified by investigating the locations of the samples with the ln k in the south section. The samples with the six greatest ln k in the south section are from four elevations and four different cores. Hence, the reason for the significant difference between the south section ln *k* and the values determined for the central and north sections is unknown.

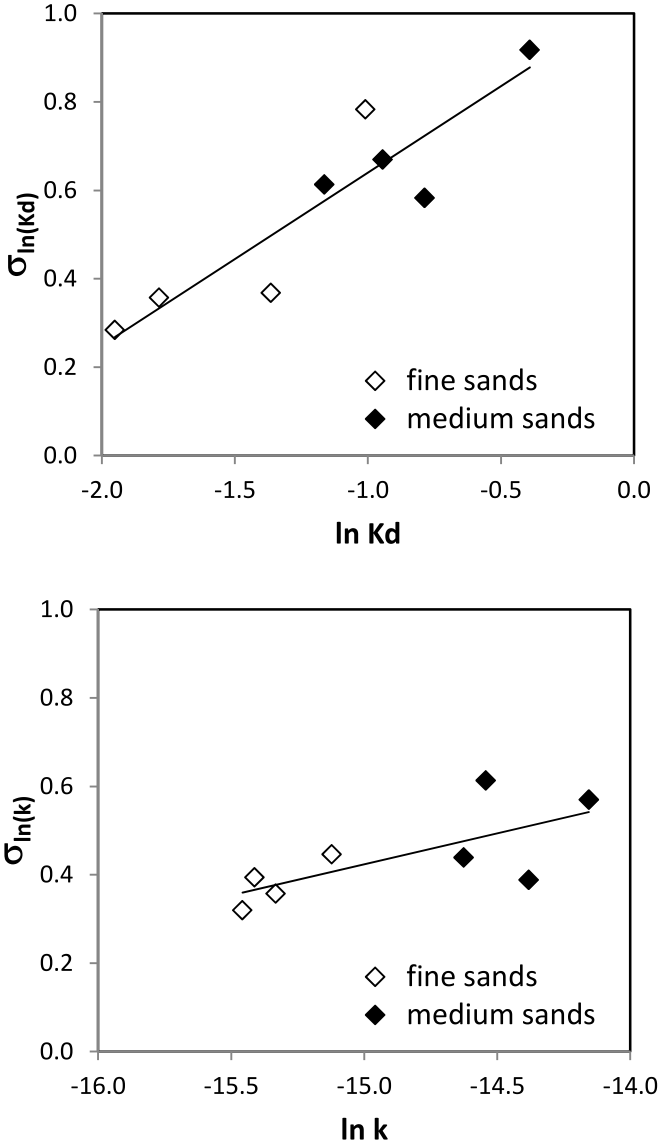


Figure S8. The correlation between the mean and standard deviation of ln K_d of the sand units is significant (a), but is not significant for ln k (b).

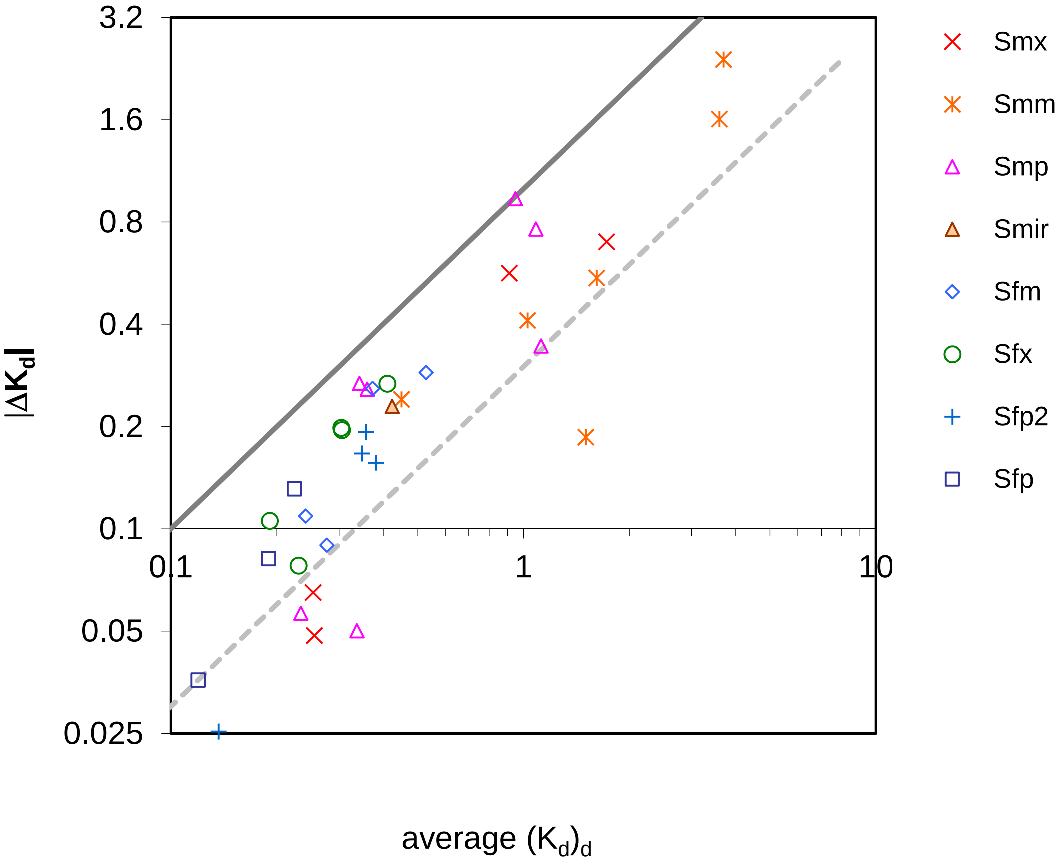


Figure S9. Absolute differences between duplicate K_d analyses plotted by unit. Lines are provided as guides: solid line is 1:1 and dashed line is $|(\Delta K_d)_d| = 0.3(\overline{K_d})_d$.

This study (1)	(2)	(3)
S_mx	HPXS	MLD
S_mx_2	MXL	MLD
S_mp	MPF	MLF
S_mm	MCG	MM
S_mir	Mottled	MLD
S_mx_3	LPXS	FLD
S_fx	XSS	FLD
S_fp	DPL	FLD
S_fp_2	FPL	FLF
S_fx_2	FPXS	FLF
S_fm	MFG	FM
Z	Z	Z
DS	DS	

Table S1. Lithofacies or unit code equivalencies between different manuscripts and/or theses.

1. Used in this manuscript (Table 1)
2. Original codes. Used by [*Allen-King et al.*, 1998], [*Divine*, 2002], [*Taylor*, 2004] [*Ritzi R.W., Jr. and Allen-King*, 2007], [*Kalinovich et al.*, 2012], and in the working portion of this study. We recognized that the units delineated by *Divine* [2002] as XSS and CPXS were the same unit viewed from different core rotation angles; these units were consolidated and delineated XSS (S_fx) in this study.
3. As used by [*Ramanathan et al.*, 2010] and [*Ritzi R. W., Jr. et al.*, 2013].

Table S2. Indicator data. Data is in separate file (2014WR016161-ts02.txt). The column headings for the data file are listed below.

1. northing (m), synonymous with core #
2. elevation MASL, meters above mean sea level
3. Working code HPXS / lithofacies S_mx, 1 when present at location
4. MCG / S_mm
5. Mottled / $S_m$ir
6. MPF / S_mp
7. MXL / S_mX_2
8. CPXS or XSS / S_fx
9. XSS or CPXS / S_fx
10. LPXS / S_mx_3
11. FPXS / S_fx_2
12. FPL / S_fp_2
13. DPL / S_fp
14. MFG / S_fm
15. Z
16. DS

Table S3. The k and K_d results, and unit, by core and sample number for the data set presented in this manuscript. Data is in separate file (2014WR016161-ts03.txt). The column headings for the data file are listed below. Abbreviations used in the table are: nd=not determined, na=not applicable. Experiment set 19 was completed using some 10 ml and some 5 ml ampoule systems, designated 19.1 and 19.5, respectively. Experiment 20 is synonymous with experiment 19.5. Abbreviations used in the table are: nd=not determined, na=not applicable

1. northing (m), synonymous with core #
2. k sample no. (tape depth relative to core-specific datum, ft)
3. elevation MASL, meters above mean sea level
4. indicator unit code
5. k, permeability, in cm2 per s
6. K_d in L per kg
7. K_d experiment set no. If multiple numbers are reported then the value is the duplicate average. DD are data from Divine (2002).
8. K_d sample no. If >1, the K_d sample is from a different location than the k sample. If > 1, the tape depth , in ft, of the K_d sample is given
9. If y, samples was selected for the unbiased data set
10. If x, K_d excluded from statistical analysis because of analytical bias

Table S4a.

	S_mx	**S_mm**	**S_fx**	**S_fp_2**	**S_fp**	**S_fm**	**Z**	**DS**	**S_mir**	**S_mp**	**All**
All data											
n	41	42	81	69	26	19	8	15	32	36	369
mean	-0.90	-0.43	-1.37	-1.75	-1.85	-1.07	-0.55	-1.44	-1.26	-0.83	-1.22
median	-0.95	-0.60	-1.43	-1.85	-1.87	-1.10	-0.57	-1.40	-1.38	-0.93	-1.34
stdev	0.75	0.82	0.35	0.48	0.34	0.66	0.54	0.33	0.52	0.66	0.71
skewness	0.47	0.38	0.37	1.90	0.45	1.45	0.06	-0.20	1.41	0.76	1.05
South section											
n	22	10	18	15	11	7	1	2	0	9	
mean	-1.08	-0.20	-1.20	-1.66	-1.92	-0.72	-0.58	-1.19		-0.84	
median	-1.03	-0.45	-1.13	-1.77	-2.00	-0.63	-0.58	-1.19		-0.77	
stdev	0.55	0.80	0.30	0.42	0.31	0.89		0.29		0.66	
skewness	0.60	0.89	-0.78	0.56	1.33	0.93				-0.13	
Central section											
n	16	28	42	46	14	10	6	7	22	23	
mean	-0.66	-0.40	-1.42	-1.77	-1.81	-1.25	-0.39	-1.56	-1.40	-0.81	
median	-0.64	-0.45	-1.47	-1.94	-1.82	-1.31	-0.50	-1.69	-1.49	-0.91	
stdev	0.97	0.84	0.32	0.53	0.37	0.39	0.45	0.31	0.38	0.57	
skewness	-0.11	0.08	0.65	2.05	0.15	-0.26	1.29	0.42	0.41	0.95	
North section											
count	3	4	21	8	1	2	1	5	10	4	
mean	-0.94	-1.19	-1.42	-1.84	-1.54	-1.41	-1.50	-1.44	-0.97	-0.94	
median	-1.00	-1.23	-1.55	-1.92	-1.54	-1.41	-1.50	-1.39	-1.27	-1.38	
stdev	0.59	0.16	0.40	0.19		0.59		0.34	0.67	1.19	
skewness	0.48	1.07	0.80	0.61				0.99	1.22	1.81	

Table S4b.

	S_mx	**S_mm**	**S_fx**	**S_fp_2**	**S_fp**	**S_fm**	**Z**	**DS**	**$S_m$ir**	**S_mp**	**All**
	All data										
n	42	42	82	78	39	19	8	13	33	40	396
mean	-14.6	-14.3	-15.4	-15.4	-15.4	-15.3	-16.1	-15.2	-14.4	-14.7	-15.0
median	-14.5	-14.2	-15.4	-15.4	-15.4	-15.4	-15.6	-15.3	-14.3	-14.8	-15.1
stdev	0.6	0.5	0.3	0.4	0.4	0.5	0.9	0.4	0.4	0.5	0.6
skewness	-0.1	-0.1	0.6	0.3	-0.2	0.4	-1.1	0.4	-0.1	0.4	0.3
	South section										
n	22	10	18	24	25	7	1	2	0	9	
mean	-14.6	-14.4	-15.2	-15.2	-15.3	-14.8	-15.3	-14.8		-14.7	
median	-14.6	-14.4	-15.3	-15.2	-15.3	-14.8	-15.3	-14.8		-14.6	
stdev	0.7	0.7	0.5	0.4	0.4	0.3		0.2		0.4	
skewness	0.2	0.1	0.3	-0.1	-0.5	0.4				-0.2	
	Central section										
n	16	28	42	45	13	10	6	6	22	24	
mean	-14.4	-14.2	-15.5	-15.4	-15.6	-15.6	-16.3	-15.3	-14.4	-14.7	
median	-14.3	-14.2	-15.5	-15.4	-15.7	-15.7	-16.1	-15.3	-14.3	-14.8	
stdev	0.5	0.4	0.2	0.3	0.4	0.2	0.9	0.3	0.5	0.5	
skewness	-0.2	0.2	0.1	-0.1	0.5	-0.5	-0.6	0.0	-0.2	0.6	
	North section										
count	4	4	22	9	1	2	1	5	11	7	
mean	-15.0	-14.5	-15.5	-15.4	-15.2	-15.4	-15.5	-15.3	-14.4	-14.9	
median	-14.9	-14.4	-15.4	-15.5	-15.2	-15.4	-15.5	-15.5	-14.4	-15.0	
stdev	0.6	0.5	0.4	0.4		0.4		0.6	0.4	0.7	
skewness	-0.9	-0.5	-0.2	1.2				1.0	0.3	1.0	

Table S4c.

	S_mx	**S_mm**	**S_fx**	**$S_f$$p_2$**	**S_fp**	**S_fm**	**Z**	**DS**	**$S_m$ir**	**S_mp**
All data										
n	32	23	44	39	13	12	8	14	18	23
mean	-0.9	-0.4	-1.4	-1.8	-2.0	-1.0	-0.6	-1.5	-1.2	-0.8
median	-0.9	-0.4	-1.5	-1.8	-2.0	-1.1	-0.6	-1.4	-1.3	-0.8
stdev	0.7	0.9	0.4	0.4	0.3	0.8	0.5	0.3	0.6	0.6
skewness	0.5	0.1	0.4	1.0	0.7	1.3	0.1	-0.1	1.2	0.1
South section										
n	22	10	10	15	10	7	1	2	0	9
mean	-1.08	-0.20	-1.20	-1.66	-1.99	-0.72	-0.58	-1.19		-0.84
median	-1.03	-0.45	-1.05	-1.77	-2.02	-0.63	-0.58	-1.19		-0.77
stdev	0.55	0.80	0.35	0.42	0.22	0.89		0.29		0.66
skewness	0.60	0.89	-1.15	0.56	1.31	0.93				-0.13
Central section										
n	10	13	13	16	3	5	6	7	8	14
mean	-0.65	-0.54	-1.40	-1.88	-1.83	-1.42	-0.39	-1.56	-1.41	-0.75
median	-0.64	-0.41	-1.48	-1.96	-1.71	-1.33	-0.50	-1.69	-1.38	-0.90
stdev	0.83	1.01	0.31	0.34	0.48	0.38	0.45	0.31	0.45	0.55
skewness	-0.09	0.08	0.84	1.34	-1.02	-0.92	1.29	0.42	0.36	0.46
North section										
count	0	0	21	8	0	0	1	5	10	0
mean			-1.42	-1.84			-1.50	-1.44	-0.97	
median			-1.55	-1.92			-1.50	-1.39	-1.27	
stdev			0.40	0.19				0.34	0.67	
skewness			0.80	0.61				0.99	1.22	

Table S4d.

	S_mx	**S_mm**	**S_fx**	**S_fp_2**	**S_fp**	**S_fm**	**Z**	**DS**	**$S_m$ir**	**S_mp**
	All data									
n	32	23	44	39	13	12	8	14	18	23
mean	-14.5	-14.2	-15.4	-15.3	-15.5	-15.1	-16.1	-15.2	-14.4	-14.6
median	-14.5	-14.1	-15.4	-15.4	-15.5	-15.1	-15.6	-15.2	-14.4	-14.5
stdev	0.6	0.6	0.4	0.4	0.3	0.4	0.9	0.4	0.4	0.4
skewness	0.0	-0.6	0.5	0.6	0.1	-0.1	-1.1	0.2	0.0	0.3
	South section									
n	22	10	10	15	10	7	1	2	0	9
mean	-14.6	-14.4	-15.2	-15.1	-15.4	-14.8	-15.3	-14.8		-14.7
median	-14.6	-14.4	-15.3	-15.2	-15.5	-14.8	-15.3	-14.8		-14.6
stdev	0.7	0.7	0.6	0.4	0.3	0.3		0.2		0.4
skewness	0.2	0.1	0.1	-0.3	-0.1	0.4				-0.2
	Central section									
n	10	13	13	16	3	5	6	6	8	14
mean	-14.5	-14.0	-15.5	-15.5	-15.5	-15.6	-16.3	-15.3	-14.4	-14.6
median	-14.5	-14.0	-15.5	-15.4	-15.7	-15.5	-16.1	-15.3	-14.4	-14.5
stdev	0.5	0.4	0.1	0.2	0.3	0.2	0.9	0.3	0.4	0.5
skewness	0.0	-0.7	0.7	-0.4	1.7	-1.1	-0.6	0.0	-0.1	0.4
	North section									
count	0	0	21	8	0	0	1	6	10	0
mean			-15.5	-15.5			-15.5	-15.1	-14.3	
median			-15.4	-15.6			-15.5	-15.3	-14.4	
stdev			0.4	0.3				0.6	0.4	
skewness			-0.2	1.6				0.2	0.3	

Table S4. The descriptive statistics for ln K_d (a) and ln k (b) by unit for each section for the complete data set; and for the unbiased data set for ln K_d (c) and ln k (d) by unit and section and overall. These statistics are for the combined units and use only new measurements for ln K_d for the S_fp and S_fp_2 units.

	n		Average ln K_d		Standard deviation ln K_d			
Unit[1]	**"new"=10 ml ampoule**	**"old"= 5 ml ampoule**	**new**	**old**	**new**	**old**	**Test[2]**	**P-value**
S_fp	11	14	-1.9	-1.5	0.3	0.4	ANOVA	0.005
S_fp_2	15	12	-1.7	-1.1	0.4	0.4	M-WU	0.002
S_fx	7	11	-1.3	-1.1	0.3	0.3	ANOVA	0.416
S_mx	11	11	-1.3	-0.8	0.4	0.6	M-WU	0.042
S_mm +S_mp	8	11	-0.6	-0.4	1.0	0.7	ANOVA	0.679

[1] Units with sufficient samples in cores 5-15.5 were tested. The S_mm and S_mp were combined to allow testing.

[2] ANOVA is analysis of variance and M-WU is Mann-Whitney U test.

Table S5. Results of K_d method comparison to test for analytical bias using samples from core numbers 5-15.5. Method-related bias was evaluated by comparing ln K_d by lithofacies for sample results of the original data set to sample results of the new cores, all taken from the south section. Lithofacies with non-normal ln K_d distributions were compared using Mann-Whitney U (nonparametric) tests and all others were compared using t-tests. The ln K_d values determined by the two methods were not significantly different for the S_fx and S_mm + S_mp units. (The latter were combined for this comparison due to low sample numbers.) Significant differences in mean ln K_d were observed for the S_fp and S_fp_2 units with the 10 ml ampoule method, producing lower averages than the 5 ml ampoule method. These differences are ascribed to analytical bias (Figure S4a). The S_fp and S_fp_2 units have the lowest K_d values (~0.18 mL/g) and this result is not unexpected for these units because the method modification was intended to reduce the uncertainty and detection limit for low-sorbing samples. Surprisingly, a significant difference was observed for the S_mx facies, but cannot be attributed to analytical differences because the 10 ml ampoule method produced a greater value than determine in the prior work – contradicting that which could be explained by the analytical method (Figure S4b). Hence the trend in the results cannot be ascribed to the analytical method and instead is attributed to a combination of low sample numbers and relatively high ln K_d variance for this lithofacies compared to others, such as the S_fx. The Z and S_fm lithofacies occurred in sample numbers too low to produce an informative result and so were not tested. Additionally, the S_mir lithofacies was not present in these cores. The result of this analysis is that the S_fp and S_fp_2 measurements from the original data set are not used in the subsequent statistical data analyses while samples of all other lithofacies in the original data set are used.

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