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Organic carbon, mercury, and sediment characteristics along a land–shore transect in Arctic Alaska

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S1 Supplementary methods

S1.1 Sedimentological analysis

The sedimentological analysis included the measurement of water-/ice content, bulk density, and grain size composition.
The water-/ice content was calculated as the difference between wet and dry weight of each sample.
The bulk density (BD) was calculated using equation S1 (Strauss et al., 2012), where the porosity (n) of the soil was calculated as the ratio of the pore volume and the total volume of the samples. It was assumed that samples with a water-/ice content of ≥ 20 % were water-/ice saturated (Strauss et al., 2012), thus the water-/ice content equals the pore volume. Moreover, an ice density at -10 °C of 0.918 g cm^{-3} and a water density at 0 °C of 0.999 g cm^{-3} was used (Harvey, 2019). The dry mineral density (ρ_s) was considered to be 2.65 g cm^{-3} (Rowell, 1994).

$$BD = (n - 1) \cdot (-\rho_s) \qquad \text{(eq. S1)}$$

The first step of the grain size analysis was the preparation of the samples, by removing the contained organic matter. Therefore, a solution of 100 ml 3 % hydrogen peroxide [H_2O_2] and 4 ml 25 % ammonia [NH_3] were added to the freeze-dried samples. They were then placed on a shaker for approximately four weeks to allow for thorough mixing and reaction of the solution with the samples. During the period of four weeks, 10 ml of 30 % H_2O_2 were added to the samples daily during weekdays, while monitoring the pH to ensure it remained between 6 and 8. If the pH fell outside of this range, it was adjusted accordingly with either ammonia or concentrated acetic acid.
The next step was to rinse the samples with purified water, to remove the H_2O_2, followed by centrifugation. The supernatant liquid was then decanted, and the remaining sediment was freeze-dried and manually homogenized. For each sample, 1 g of the homogenized material was placed into a plastic container, to which 0.5 g of tetra-sodium pyrophosphate [$Na_4P_2O_7$] and 0.0001 % ammonia solution [NH_3] were added to disperse the soil particles and prevent them from settling during the subsequent analysis. The sample container was then placed on a "Gerhard Laboshake overhead shaker" for 24 hours to allow for complete dispersion of the added solution. Each sample was than split into eight subsamples with a particle concentration of 5-15 % by a rotary cone sample divider. Simultaneously all particles > 1 mm were sieved out before analysis, weighed, and included in the results at the end. The grain size measurement was carried out using a *Malvern Mastersizer 3000* with a *Malvern Hydro LV wet-sample dispersion Unit.*
The international ISO 14688-1:2017 scale was used for the grain size classification. The ranges specified there are ≤ 2 µm for clay, 2 µm to 63 µm for silt and 63 µm to 2 mm for sand (ISO 14688-1:2017, 2017). All statistics of the grain size distribution were calculated using the software GRADISTAT (Blott and Pye, 2001).

S1.2 Hydrochemical analysis

The selected samples were thawed at room temperature overnight, to prepare them for the porewater extraction. The porewater was taken the next day, using Rhizons (RHIZONS MOM 5 and 10 cm, Rhizospheres Research Products). Therefore, the Rhizons were inserted into the soil samples and a vacuum was created using plastic syringes. The extracted water was than distributed into different vials for the different hydrochemical measurements (pH value, electrical conductivity (EC), anions). The pH value and EC were measured one day after the pore water extraction with a *WTW Multilab 540* using 4 ml of porewater. The concentration of anions in the porewater can provide different information, like the availability and mobility of nutrients, as well as a potential risk of anion accumulation leading to soil degradation. In this study, the chloride and sulfate concentrations are of particular interest, as they provide information on the degree of acidification and salinization and can thus indicate the extent to which the sample sites are influenced by the ocean.
For the measurement of anions 5 ml of the pore water of every sample was filled into an 8 ml LDPE-Bottle. Samples with a high electrical conductivity were diluted in ratio of 1:25, 1:50 or 1:100, where applied the higher the electrical conductivity the higher the dilution ratio. The Anions were measured using a *Thermo ICS2100*. For the analysis of the DOC content in the

porewater 10-20 ml of each sample was filled into a glass vial. To preserve the samples until further analysis they were acidified with 50 µl of 30 % hydrochloric acid (HCL) and stored at 4 °C. The measurement was carried out using a *Shimadzu Total Organic Carbon Analyzer (TOC-VCPH)*. The results of three to five injections were used as an average to determine the total DOC content. The detection limit was 0.25 mg/L and the uncertainty ranged between ±10 % for measured values higher than 1.5 mg/L and ±15-20 % for values lower than 1.5 mg/L.

S2 Supplementary figures

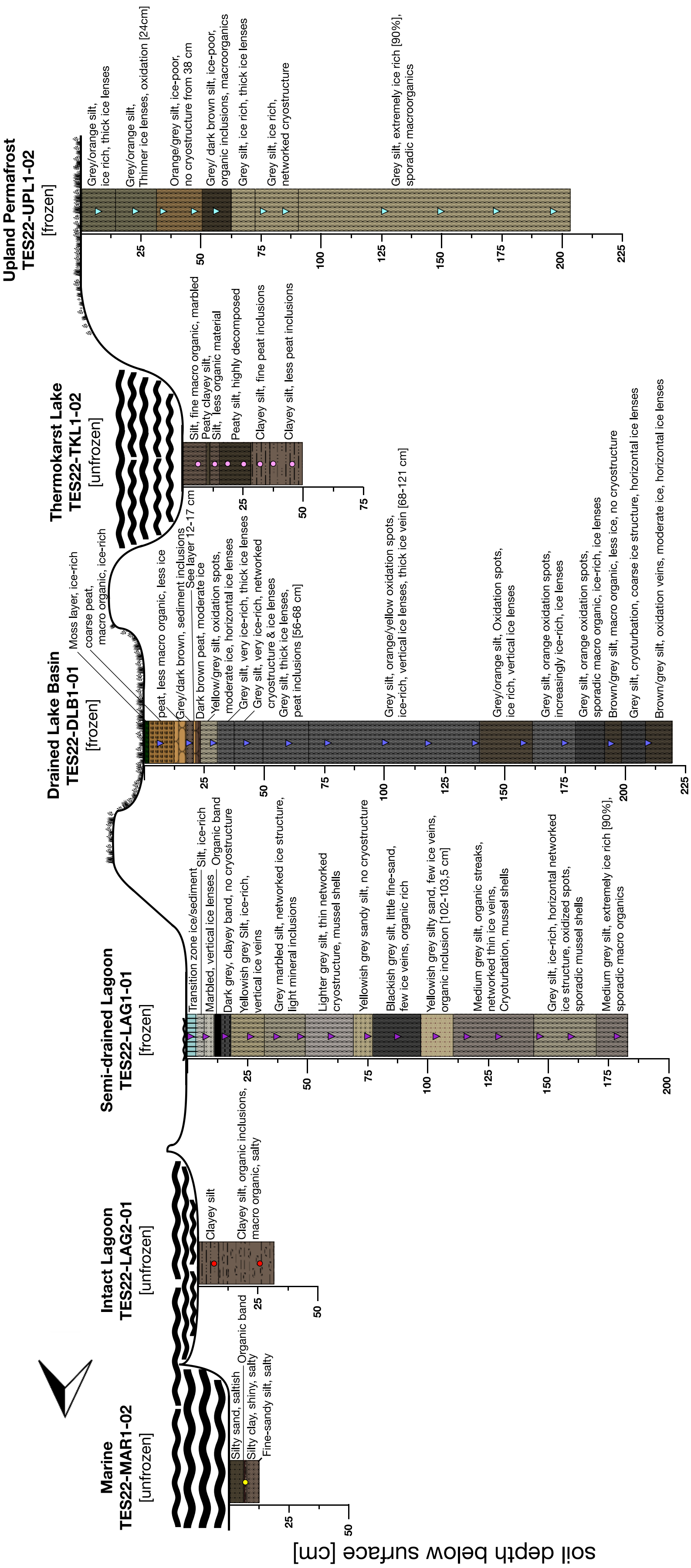

Figure S1: Stratigraphic core description of the soil profiles. Samples marked as points (unfrozen sediments) and triangles (frozen sediments). Core abbreviations: UPL: upland permafrost, TKL: thermokarst lake, DLB: drained lake basin, SDLAG: semi-drained lagoon, LAG: lagoon, MAR: marine.

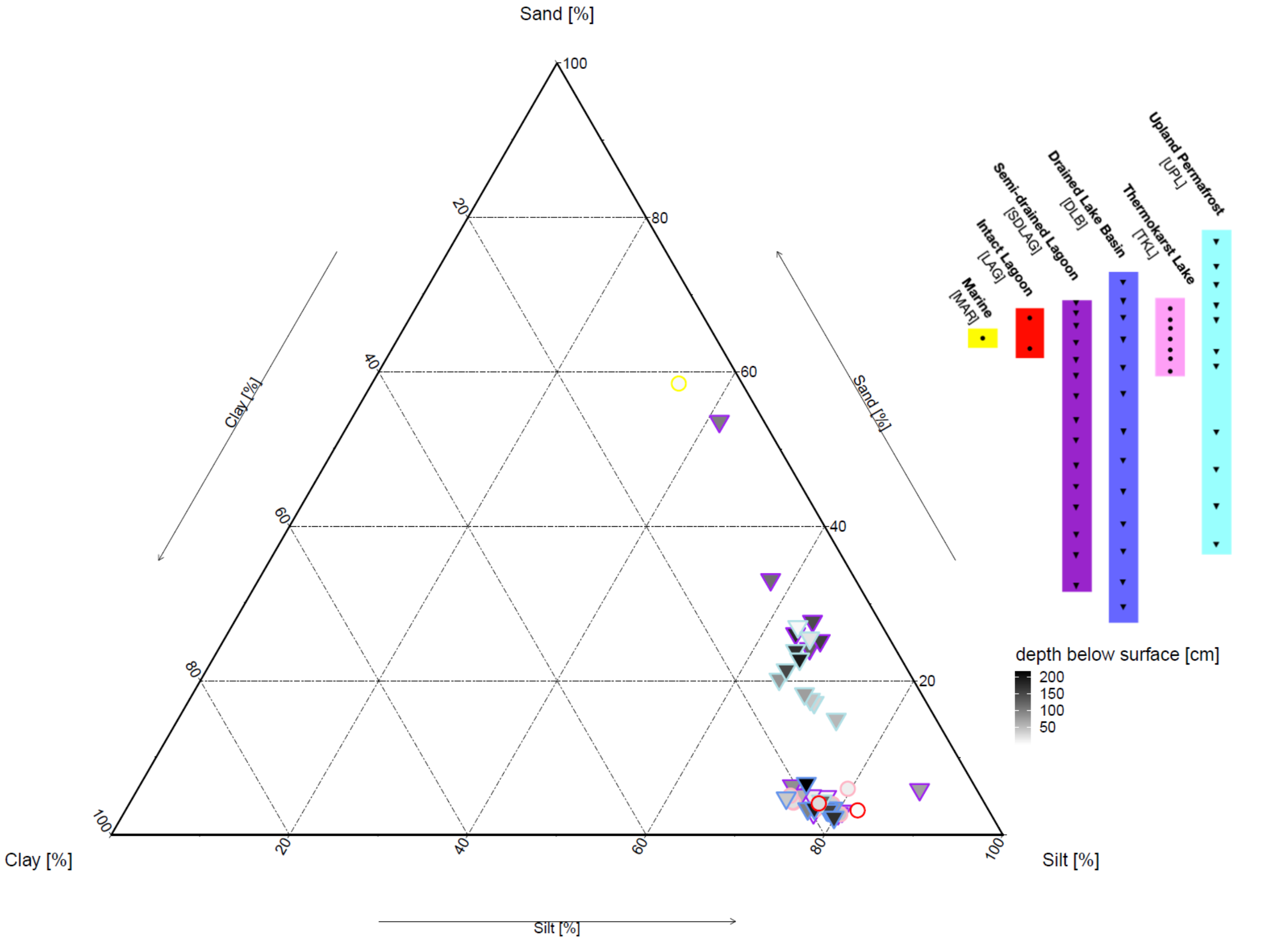

Figure S2: Soil triangle showing the grainsize distribution of the soil profiles, with circles for unfrozen sediments and triangles for frozen sediments and a colour gradient over depth below surface [cm]. Core abbreviations: UPL: upland permafrost, TKL: thermokarst lake, DLB: drained lake basin, SDLAG: semi-drained lagoon, LAG: lagoon, MAR: marine.

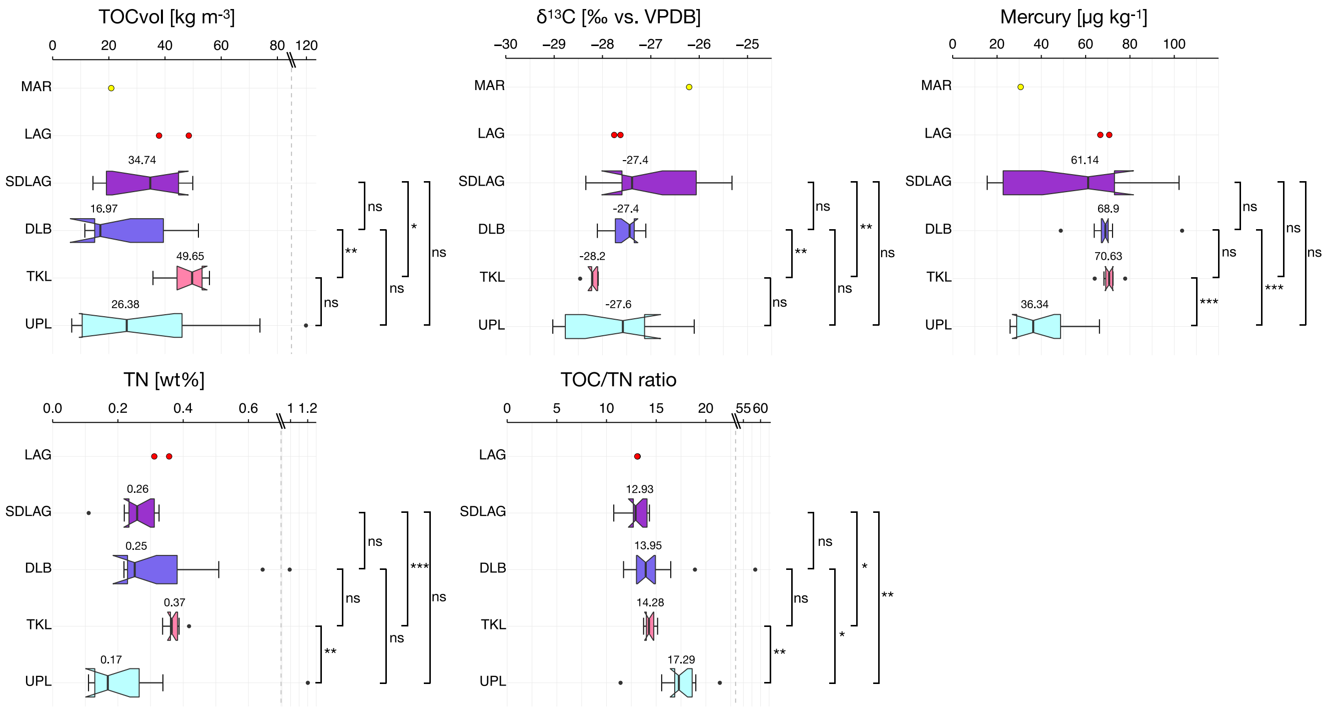

Figure S3: Boxplots of the biogeochemical parameters: total organic carbon density (TOCvol), stable carbon isotope ratio ($\delta^{13}C$), mercury, total nitrogen (TN), and total organic carbon/ nitrogen (TOC/TN) ratio of the SDLAG, DLB, TKL, and UPL profiles and MAR and LAG as individual samples. The whiskers display the data range (outliers as black points) and the boxes show the interquartile range (25-75 %). The black vertical line marks the median and the notches represent the 95 % confidence interval. The bars right of the boxes show the statistical significance of differences between the profiles (ns = not significant; * = $p < 0.05$; ** = $p < 0.01$; *** = $p < 0.001$). Core abbreviations: UPL: upland permafrost; TKL: thermokarst lake; DLB: drained lake basin; SDLAG: semi-drained lagoon; LAG: lagoon; MAR: marine. Split x axis for TOCvol, TN, TOC/TN ratio.

S3 Supplementary tables

Table S1: Results of the Hydrochemical analysis. Core abbreviations: UPL: upland permafrost; TKL: thermokarst lake; DLB: drained lake basin; SDLAG: semi-drained lagoon; LAG: lagoon; MAR: marine.

Hydrochemical Analysis	Mean depth [cm]	pH value	Electrical conductivity [mS cm^{-1}]	DOC as NPOC [mg l^{-1}]
MAR	6.25	7.67	39.5	19.2
LAG	5	7.64	54.6	NA
SDLAG	7.75	7.49	39.0	80.8
SDLAG	87	5.94	61.5	NA
SDLAG	179	7.58	17.85	NA
DLB	6.75	4.52	0.26	52.3
DLB	60.5	6.99	0.67	187
DLB	215	6.61	0.33	378
TKL	6	7.45	0.83	NA
UPL	7	6.44	0.31	72.3
UPL	56	7.32	0.36	NA
UPL	195	7.25	0.12	228

S4 Supplementary R-scripts

S4.1 R-script Kruskal-Wallis rank sum test

```
### required packages
library("psych")
library("rstatix")
library("dplyr")
library("readxl")
### load data
kw_data <- read_excel("/…kw_data.xlsx")
# descriptive statistic by group
describeBy(kw_data$Parameter,kw_data$Prefix)
### using Kruskal-Wallis-Test
kruskal.test(kw_data$Parameter~kw_data$Prefix)
# example result: Kruskal-Wallis chi-squared = 11.131, df = 3, p-value = 0.01104
### post-hoc analyse (dunn's test)
dunn_test(Parameter~Prefix, data=kw_data, p.adjust.method = "bonferroni")
```

S4.2 R-script Mann-Whitney-Wilcoxon test

```
### required packages
library("psych")
library("readxl")
### Mann-Whitney-U-Test pairwise site comparison
### load data pairwise
data_two_cores <- read_excel("/…core_1-core_2.xlsx")
### calculate Mann-Whitney-U-Test
wilcox.test(parameter~Prefix, data = data_two_cores, exact = TRUE, correct = FALSE, conf.int = FALSE)
```

```
# example results: p-value = 0.01154
### effect size
z_parameter <- qnorm(p-value/2)
# print z-value
z_parameter
# example result: z = -2.525907
r_parameter <- z_parameter/sqrt(49)
# print r-value
r_parameter
#  example result: 0.3608439
### Mann-Whitney-U-Test comparison frozen vs. unfrozen
### load data
fn_data <- read_excel("/..fro_unfro.xlsx")
### descriptive statistic by groups
describeBy(fn_data$parameter,fn_data$Prefix)
# example result: frozen: mean = 4.76 wt%, median = 5.1  ; unfrozen: mean = 4.75 wt%, median 3.17
### calculate Mann-Whitney-U-Test
wilcox.test(parameter~Prefix, data = fn_data, exact = FALSE, correct = FALSE, conf.int = FALSE)
#example result: p-value = 0.007946
### effect size
z_parameter <- qnorm(p-value/2)
# print z-value
z_paramter
# example result: z = -2.654356
r_parameter <- z_parameter/sqrt(49)
# pront r-value
r_parameter
# example result: 0.3791937
### same procedure for saline/non-saline comparison
```

S4.3 R-script Correlation matrix

```
### required packages
library("corrplot")
library("readxl")

### load data
cm_data <- read_excel("/…correlation_matrix.xlsx")
### create correlation matrix
Correlationm <- cor(cm_data)
### create correlation matrix with p-value
Correlationp <- cor.mtest(cm_data)
### start the plot
pdf(file = "/… /correlations_matrix.pdf",
```

```
    width = 20,
    height = 20)
### plot with numbers
corrplot(Correlationm, method = "number", p.mat=Correlationp$p, insig = "blank",
         tl.col = "black", tl.srt = 59, tl.cex = 3,
         number.cex = 2, label.srt = 50)
### add the second half of the plot as dots
corrplot(Correlationm, p.mat=Correlationp$p, insig = "blank", type = "upper", tl.pos = "n", tl.cex =1.5, add = TRUE)
### save the plot
dev.off()
```

Supplementary References

Blott, S. J. and Pye, K.: GRADISTAT: a grain size distribution and statistics package for the analysis of unconsolidated sediments, Earth Surf Processes Landf, 26, 1237–1248, https://doi.org/10.1002/esp.261, 2001.

Harvey, A.: Properties of Ice and Supercooled Water, in: CRC Handbook of Chemistry and Physics, CRC Press, Boca Raton, FL, 2019.

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