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Supporting Information for

Asymmetric patterns of soil carbon mineralization during thaw slump recovery: Stable fast-pool size but rebounding decomposition rate

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Supplementary Information Introduction

This Supplementary Information provides additional methodological details, raw data summaries, and validation results supporting the findings of the main manuscript titled "*Asymmetric patterns of soil carbon mineralization during thaw slump recovery: Stable fast-pool size but rebounding decomposition rate*". It includes 15 tables (S1–S15), 3 figures (S1–S3), and one technical note (Note S1), organized as follows:

Tables S1–S3 describe the measured soil properties, analytical methods, and Python libraries used for data processing and modeling, ensuring reproducibility of all statistical procedures.

Tables S4–S9 present model selection criteria (AICc), goodness-of-fit metrics, and partial least squares structural equation modeling (PLS-SEM) results—including path coefficients, effect decompositions, permutation tests, and predictive relevance (Q^2)—to validate the causal relationships between restoration time, organic carbon chemistry, microbial biomass, and k_{fast}.

Tables S10–S11 extend the PLS-SEM framework by incorporating soil organic carbon $\delta^{13}C$ and pH as additional drivers, and report correlation matrices linking soil moisture, texture, and carbon mineralization parameters.

Tables S12–S15 detail sensitivity analyses of the two-pool model's parameter upper bounds, two-way ANOVA results under varying constraints, and robustness checks excluding single-pool samples, confirming that core conclusions are not biased by modeling choices.

Figures S1–S3 visualize key bivariate relationships: a correlation heatmap of soil carbon, chemistry, and microbial metrics (S1); the negative trend of $\delta^{13}C$ with restoration time and its link to k_{fast} (S2); and the recovery of soil pH and its positive association with k_{fast} (S3).

Note S1 provides a technical justification for the selected upper bounds of the two-pool model parameters ($k_{fast} \leq 1.0$ d^{-1}, $k_{slow} \leq 0.5$ d^{-1}), demonstrating their validity and robustness.

Together, these materials reinforce the main text's conclusions by addressing methodological transparency, statistical rigor, and the independence of key findings from analytical assumptions.

Table S1. Summary of measured soil physicochemical properties, carbon chemical composition, microbial characteristics, and extracellular enzyme activities, including units and notes.

Variable Category	Specific Variables	Unit / Notes
Soil Physicochemical Properties	Soil Organic Carbon (SOC) content	g/kg
	Total Nitrogen (TN) content	g/kg
	Carbon to Nitrogen ratio (C/N)	Ratio
	Dissolved Organic Carbon (DOC)	mg/kg
	Soil Water Content	%
	pH	Unitless
	Clay content	%
	Silt content	%
	Sand content	%
Carbon Chemistry Structure (^{13}C NMR)	Alkyl C	%
	O-alkyl C	%
	Aromatic C	%
	Carboxyl C	%
	Alkyl C / O-alkyl C ratio	Ratio
Microbial Community (PLFA)	Total PLFA	μg/g
	Fungal PLFA	μg/g
	Bacterial PLFA	μg/g
	Actinobacterial PLFA	μg/g
	Fungal to Bacterial ratio (F/B)	Ratio
Extracellular Enzyme Activities	β-1,4-Glucosidase (BG)	nmol/g/h
	β-1,4-N-Acetylglucosaminidase (NAG)	nmol/g/h
	Leucine Aminopeptidase (LAP)	nmol/g/h
	Acid Phosphatase (MUF-Phos)	nmol/g/h
Cumulative CO_2 Release	Cumulative CO_2 release	mg CO_2-C/g SOC

Table S2. List of Python libraries and modules used in this study with corresponding analytical purposes.

Library / Module	Purpose
pandas	Data reading, processing, and merging
numpy	Numerical computation and array manipulation
matplotlib.pyplot	Plotting and graphical styling
seaborn	Statistical chart generation and beautification
scipy.optimize	Nonlinear least-squares fitting (curve_fit)
scipy.stats	Statistical tests (Pearson correlation, normal distribution, etc.)
sklearn.decomposition	Principal component analysis (PCA)
sklearn.preprocessing	Data standardization (StandardScaler)
sklearn.linear_model	Linear regression (LinearRegression)
sklearn.cross_decomposition	Partial least squares regression (PLSRegression)
itertools	Generation of combinations (used in hierarchical partitioning)
statsmodels.api	Analysis of variance (ANOVA) and statistical modeling
statsmodels.formula.api	R-style formula interface (OLS)
statsmodels.stats.multicomp	Post-hoc multiple comparison (Tukey HSD)
warnings	Suppression of warning messages

Table S3. Comparison of model fit between the single-pool and two-pool models for each soil sample (AICc and R^2).

SampleID	Years	Depth	AICc single	AICc double	Delta AICc	Selected model	R^2
1-C-A1	Control	Topsoil	12.1	-35.4	47.6	double	0.998
1-C-A2	Control	Topsoil	5.16	-46.4	51.5	double	0.997
1-C-A3	Control	Topsoil	-2.29	-54.9	52.6	double	0.997
1-HT1-A1	1 year	Topsoil	-1.58	-55.4	53.8	double	0.998
1-HT1-A2	1 year	Topsoil	5.61	-47.1	52.7	double	0.998
1-HT1-A3	1 year	Topsoil	6.00	-49.4	55.4	double	0.995
1-HT2-A1	12 years	Topsoil	1.73	-54.4	56.1	double	0.998
1-HT2-A2	12 years	Topsoil	7.93	-50.9	58.9	double	0.998
1-HT2-A3	12 years	Topsoil	-4.99	-65.7	60.7	double	0.996
1-HT3-A1	23 years	Topsoil	-39.5	-33.8	-5.70	single	0.955
1-HT3-A2	23 years	Topsoil	-20.4	-70.0	49.6	double	0.998
1-HT3-A3	23 years	Topsoil	-47.9	-65.0	17.2	double	0.994
1-C-B1	Control	Subsoil	-36.6	-82.0	45.4	double	0.999
1-C-B2	Control	Subsoil	-25.3	-74.4	49.1	double	0.999
1-C-B3	Control	Subsoil	-26.6	-64.0	37.4	double	0.997
1-HT1-B1	1 year	Subsoil	-35.3	-81.1	45.8	double	0.999

1-HT1-B2	1 year	Subsoil	2.50	-43.7	46.2	double	0.997
1-HT1-B3	1 year	Subsoil	-14.5	-58.1	43.6	double	0.996
1-HT2-B1	12 years	Subsoil	-27.8	-77.0	49.2	double	0.998
1-HT2-B3	12 years	Subsoil	-35.3	-67.6	32.3	double	0.994
1-HT3-B1	23 years	Subsoil	-61.4	-91.3	30.0	double	0.999
1-HT3-B2	23 years	Subsoil	-61.4	-65.4	4.02	double	0.997
1-HT3-B3	23 years	Subsoil	-49.2	-59.6	10.4	double	0.992

Table S4. Effect sizes (Cohen's d) of k_{fast} comparing the stable stage (23 years) with other restoration stages.

Comparison	Cohen's d
23 years vs 1 year	1.94
23 years vs 12 years	1.45
23 years vs Control	1.67

Table S5 Pearson correlation matrix and significance levels (*p*) among soil carbon pool parameters, chemical properties, and microbial traits.

	$C_{0,total}$	$C_{0,fast}$	k_{fast}	$C_{0,slow}$	k_{slow}	SOC	TN	C/N	DOC	O-alkyl C	Alkyl C	Alkyl C/O-alkyl C	PLFA	F PLFA/B PLFA	BG	NAG
$C_{0,total}$	1.00															
$C_{0,fast}$	0.029	1.00														
k_{fast}	0.001	0.009	1.00													
$C_{0,slow}$	0.000	0.029	0.001	1.00												
k_{slow}	0.002	0.014	0.005	0.002	1.00											
SOC	0.227	0.187	0.071	0.227	0.569	1.00										
TN	0.768	0.595	0.167	0.768	0.800	0.001	1.00									
C/N	0.106	0.173	0.535	0.106	0.569	0.403	0.290	1.00								
DOC	0.222	0.145	0.060	0.222	0.683	0.440	0.417	0.929	1.00							
O-alkyl C	0.162	0.000	0.092	0.162	0.105	0.058	0.316	0.158	0.484	1.00						
Alkyl C	0.235	0.024	0.045	0.235	0.011	0.850	0.443	0.290	0.477	0.141	1.00					
Alkyl C/O-alkyl C	0.158	0.003	0.023	0.158	0.007	0.465	0.306	0.602	0.411	0.016	1.71E-08	1.00				
PLFA (Total)	0.249	0.003	0.209	0.249	0.354	0.298	0.603	0.389	0.086	0.118	0.312	0.206	1.00			
F PLFA/B PLFA	0.412	0.017	0.356	0.412	0.303	0.691	0.610	0.073	0.201	0.004	0.430	0.168	0.299	1.00		
BG	0.138	0.348	0.466	0.138	0.776	0.534	0.926	0.182	0.766	0.913	0.620	0.655	0.230	0.646	1.00	
NAG	0.095	0.181	0.375	0.095	0.518	0.592	0.878	0.200	0.593	0.793	0.419	0.458	0.081	0.827	9.40E-10	1.00

Table S6. Bootstrap-based significance test results for path coefficients in the PLS-SEM.

From	To	CI lower	CI upper	p	Significance
Recovery Time	Organic Chemistry	0.062	1.07	0.035	*
Recovery Time	Microbial Biomass	-2.18	-0.223	0.022	*
Organic Chemistry	Microbial Biomass	-1.90	0.360	0.132	ns
Recovery Time	k_{fast}	0.142	1.12	0.005	**
Organic Chemistry	k_{fast}	0.241	1.10	0.008	**
Microbial Biomass	k_{fast}	-0.456	-0.033	0.141	ns

Table S7. Decomposition of the total, direct, and indirect effects of restoration age on k_{fast}.

Effect	Coefficient
Direct	0.697
Indirect (via Organic Chemistry)	0.328
Indirect (via Microbial Biomass)	0.217
Indirect (serial)	0.093
Total Indirect	0.639
Total Effect	1.34

Table S8. Permutation test results for path coefficients in the PLS-SEM.

From	To	Original coef	Permuted mean	Permuted std	Permutation p	Perm CI lower	Perm CI upper
Recovery Time	Organic Chemistry	0.541	-0.002	0.277	0.047	-0.545	0.523
Recovery Time	Microbial Biomass	-1.16	-0.003	0.556	0.028	-1.03	1.08
Organic Chemistry	Microbial Biomass	-0.920	0.010	0.555	0.094	-1.13	0.988
Recovery Time	k_{fast}	0.697	1.94E-04	0.278	0.005	-0.516	0.540
Organic Chemistry	k_{fast}	0.607	-0.001	0.277	0.021	-0.557	0.488
Microbial Biomass	k_{fast}	-0.188	-0.001	0.138	0.167	-0.219	0.292

Table S9. Predictive relevance (Q^2) assessment for the Partial Least Squares Structural Equation Model (PLS-SEM).

Latent Variable	Q^2	PRESS	SSO
Organic Chemistry	0.173	32.9	39.8
Microbial Biomass	0.0125	81.4	82.5
k_{fast}	0.349	13.2	20.2

Table S10. Extended partial least squares structural equation model (PLS-SEM) path coefficients incorporating soil organic carbon δ^{13}C and pH as additional latent variables

From	To	Coefficient	CI lower	CI upper	p	Significance
Recovery Time	Organic Chemistry	0.541	0.072	1.08	0.033	*
Recovery Time	Carbon Isotope	-0.761	-1.11	-0.393	0.000	***
Recovery Time	Acidity	0.152	-0.390	0.658	0.556	ns
Recovery Time	Microbial Biomass	-1.158	-2.20	-0.244	0.024	*
Organic Chemistry	Carbon Isotope	-0.700	-1.11	-0.317	0.000	***
Organic Chemistry	k_{fast}	0.607	0.248	1.12	0.008	**
Carbon Isotope	k_{fast}	-0.572	-1.05	-0.163	0.015	*
Acidity	Microbial Biomass	-0.653	-1.51	0.027	0.095	ns
Acidity	k_{fast}	0.515	0.155	1.22	0.041	*
Microbial Biomass	k_{fast}	-0.188	-0.459	-0.032	0.209	ns
Recovery Time	k_{fast}	0.697	0.140	1.11	0.005	**

Table S11. Pearson correlation matrix among soil moisture, texture, and fast-pool decomposition rate constant (k_{fast})

	Moisture	Clay1	Silt	Clay2	k_{fast}	$C_{0,fast}$	A/O
Moisture	1.00	0.351	0.073	-0.183	-0.360	0.114	-0.360
Clay1	0.351	1.00	0.073	-0.396	-0.041	-0.068	0.024
Silt	0.073	0.073	1.00	-0.945	-0.305	0.037	-0.243
Clay2	-0.183	-0.396	-0.945	1.00	0.294	-0.012	0.212
k_{fast}	-0.360	-0.041	-0.305	0.294	1.00	-0.671	0.624
$C_{0,fast}$	0.114	-0.068	0.037	-0.012	-0.671	1.00	-0.758
A/O	-0.360	0.024	-0.243	0.212	0.624	-0.758	1.00

Table S12. Fraction of samples reaching the upper bound of k_{fast} under different upper bound values (with k_{slow} bound fixed at 0.5 d^{-1}).

k_{fast} upper bound (d^{-1})	Fraction at the bound
0.5	0.217
1.0	0.174
2.0	0.130
5.0	0.130
1,000,000 (unconstrained)	0.0000

Table S13. Fraction of samples reaching the upper bound of k_{slow} under different upper bound values (with k_{fast} bound fixed at 1.0 d^{-1}).

k_{slow} upper bound (d^{-1})	Fraction at the bound
0.2	0.0
0.5	0.0
1.0	0.0
2.0	0.0

Table S14. Two-way ANOVA results for k_{fast} under different upper bounds of k_{fast} (Years: recovery year; Depth: soil depth).

k_{fast} upper bound (d^{-1})	Years *p*	Depth *p*	Years × Depth *p*	*N*
0.5	0.028	0.045	0.833	23
1.0	0.003	0.218	0.942	23
2.0	0.003	0.413	0.993	23
5.0	0.008	0.445	0.866	23

Table S15. Robustness check of core statistical results after excluding the sample fitted by the single-pool model.

Analysis item	All samples	Double-library samples	Consistent?
ANOVA p-value (Years for k_{fast})	0.0135	0.0135	Yes
Pearson r (k_{fast} vs. Alkyl/O-alkyl)	0.624	0.624	Yes
p-value (k_{fast} vs. Alkyl/O-alkyl)	0.0130	0.0130	Yes
LMG: Total contribution of organic chemistry quality	0.299	0.299	Yes
PLS path coefficient: Recovery Time $\rightarrow k_{fast}$	0.697	0.697	Yes
PLS path coefficient: Organic Chemistry $\rightarrow k_{fast}$	0.607	0.607	Yes

Notes S1. Sensitivity analysis of the upper bounds for the two-pool mineralization model parameters.

To evaluate the influence of the parameter upper bounds in the two-pool model (k_{fast} ≤1.0 d⁻¹, k_{slow}≤0.5 d⁻¹) on the fitting results and conclusions, we performed a sensitivity analysis of the upper bounds. We re-fitted the two-pool model for all samples under a series of upper-bound settings: for k_{fast} , the upper bound was set at 0.5, 1.0, 2.0, and 5.0 d^{-1} with the k_{slow} bound fixed at 0.5 d^{-1}; for k_{slow} , the upper bound was set at 0.2, 0.5, 1.0, and 2.0 d^{-1} with the k_{fast} bound fixed at 1.0 d^{-1}.The results showed that the fraction of samples reaching the k_{slow} bound was 0% under all tested upper bounds, indicating that the bound of 0.5 d^{-1} is sufficiently loose and does not impose any constraint on parameter estimation.

For k_{fast} , when the upper bound was 0.5 d^{-1}, 21.7% of the samples reached the bound; this fraction decreased to 17.4% when the bound was relaxed to 1.0 d^{-1}, and stabilized at approximately 13.0% at bounds of 2.0 and 5.0 d^{-1} (Table. S2). This pattern suggests that the 1.0 d^{-1} bound exerts only a mild constraint on a small number of samples. Furthermore, two-way ANOVA confirmed that the main effect of recovery year on k_{fast} remained significant (all p<0.05) across the different k_{fast} upper bounds (0.5–5.0 d^{-1}), whereas the effects of soil depth and their interaction were not significant (Table S4). The core statistical conclusion is thus completely unaffected by the choice of the upper bound. Therefore, the parameter upper bounds adopted in this study (k_{fast} ≤1.0 d^{-1}, k_{slow} ≤0.5 d^{-1}) can prevent non-physical solutions during numerical optimization without compromising the main scientific findings, and represent a reasonable and robust choice.

Figure S1. Correlation heatmap of soil carbon, chemistry, and microbial metrics

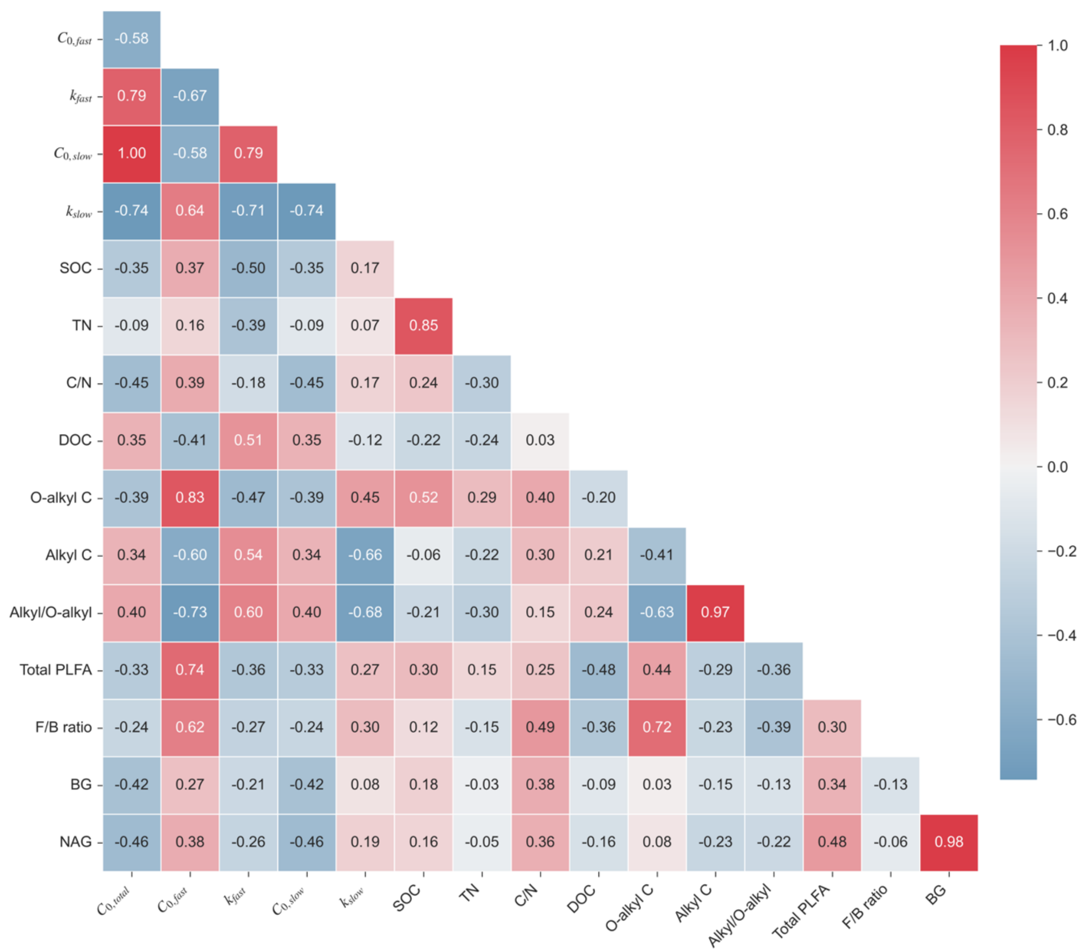

Figure S2. Relationships between soil organic carbon δ^{13}C and the alkyl C/O-alkyl C ratio (A/O) and k_{fast}

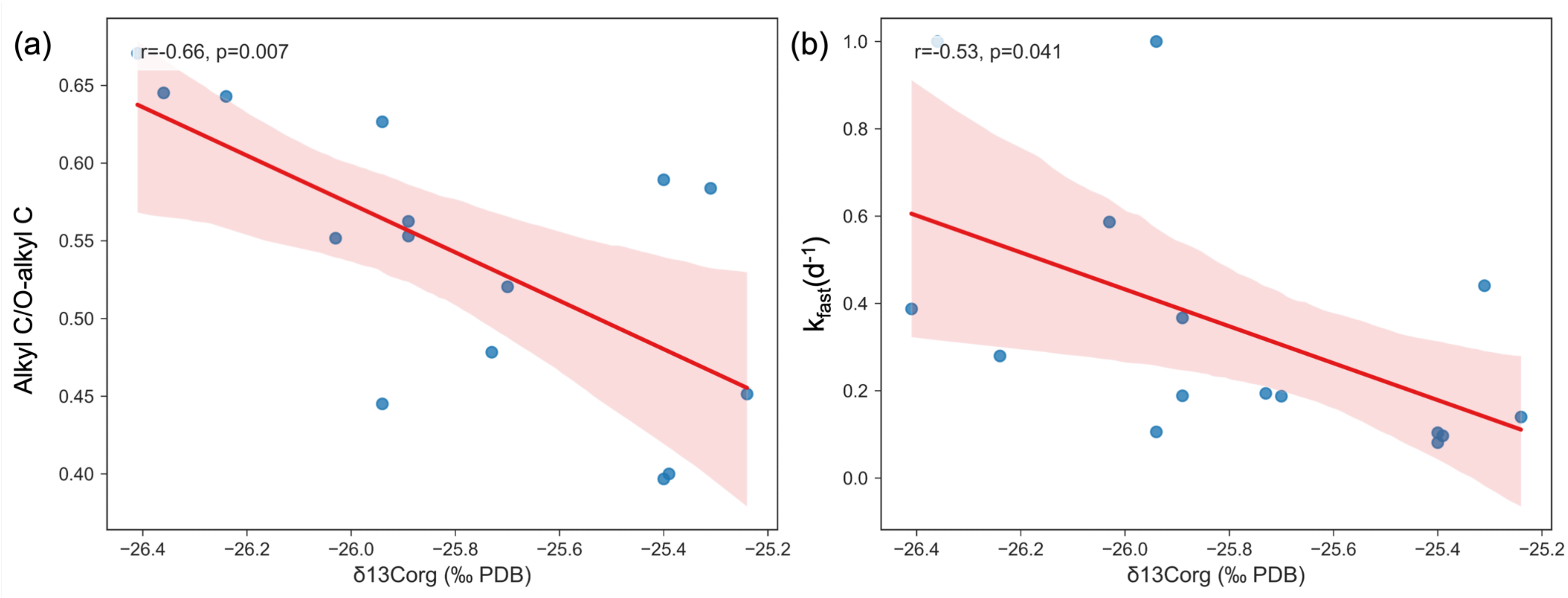

Figure S3. Relationship between soil pH and k_{fast}