

Table S1 Bulk density of 0–200 soil layers in two seasons.

Soil depth (cm)	Bulk density in S1 (g cm⁻³)	Bulk density in S2 (g cm⁻³)
0–20	1.120	1.121
20–40	1.164	1.156
40–60	1.195	1.189
60–80	1.216	1.212
80–100	1.323	1.333
100–120	1.346	1.340
120–140	1.367	1.371
140–160	1.356	1.366
160–180	1.349	1.379
180–200	1.432	1.400

Table S2 RF model performance and variable exclusion

Group	Model	p	OOB R^2 mean $\pm$ SD	OOB $RMSE$ mean $\pm$ SD	LOBO R^2	LOBO $RMSE$
B0	Original	13	0.9280 $\pm$ 0.0013	0.2902 $\pm$ 0.0027	0.919	0.308
B0	Core exclusion	9	0.8804 $\pm$ 0.0019	0.3741 $\pm$ 0.0030	0.875	0.383
B0	Strict exclusion	8	0.8486 $\pm$ 0.0026	0.4209 $\pm$ 0.0036	0.851	0.418
B0	N rate baseline	2	0.7837 $\pm$ 0.0073	0.5031 $\pm$ 0.0085	0.794	0.491
B20	Original	13	0.9669 $\pm$ 0.0007	0.2606 $\pm$ 0.0027	0.958	0.292
B20	Core exclusion	9	0.9547 $\pm$ 0.0007	0.3046 $\pm$ 0.0024	0.946	0.333
B20	Strict exclusion	8	0.9436 $\pm$ 0.0009	0.3401 $\pm$ 0.0026	0.936	0.363
B20	N rate baseline	2	0.8361 $\pm$ 0.0071	0.5796 $\pm$ 0.0125	0.840	0.574

p denotes predictor count. Original contains 13 traits. Core exclusion removes GN, HI, TransDM and PostDM; strict exclusion also removes DMM. The N rate baseline contains NR and Season only. All models use 1000 trees, nodesize 5 and mtry = floor($p/3$), with a minimum of 1.

OOB means and SDs summarize 100 random seed fits. These SDs describe algorithm variability, not sampling uncertainty. OOB R^2 uses the randomForest sample variance denominator. LOBO uses eight complete season by block holdouts, averaging each plot's predictions across 10 seed fits; pooled $R^2 = 1 - SSE/SST$. $RMSE$ is in $t\ ha^{-1}$.

B0 — Core exclusion: ΔR^2 -0.044, $RMSE$ +24.2%; Strict exclusion: ΔR^2 -0.068, $RMSE$ +35.6%; N rate baseline: ΔR^2 -0.125, $RMSE$ +59.5%.

B20 — Core exclusion: ΔR^2 -0.012, $RMSE$ +13.8%; Strict exclusion: ΔR^2 -0.023, $RMSE$ +24.2%; N rate baseline: ΔR^2 -0.119, $RMSE$ +96.3%.

Trait model versus N rate baseline performance does not estimate an N adjusted causal contribution. Performance loss cannot be assigned solely to mathematical coupling.

Table S3 RF permutation importance with whole block bootstrap intervals

Group	Model	Trait	Mean <i>MSE</i> increase (%)	95% bootstrap CI (%)
B0	O	DMM	90.72	22.43 to 204.87
B0	O	HI	21.17	8.53 to 41.52
B0	O	PostDM	180.22	58.22 to 429.17
B0	O	DMA	28.70	-3.36 to 81.09
B0	O	DMT	1.64	-5.72 to 8.98
B0	O	NUPA	24.74	-5.21 to 74.72
B0	O	PostNUP	16.24	-9.08 to 48.41
B0	O	NUPM	28.52	-8.30 to 82.23
B0	O	GW	18.03	0.30 to 49.15
B0	O	GN	69.31	7.51 to 194.47
B0	O	SWC	1.33	-2.93 to 6.09
B0	O	PostLAI _m	27.20	-8.78 to 74.37
B0	O	PostSPAD _m	11.47	-9.74 to 39.61
B0	C	DMM	127.73	33.68 to 278.06
B0	C	DMA	32.80	-4.08 to 85.64
B0	C	NUPA	29.55	-8.69 to 83.07
B0	C	PostNUP	19.62	-13.03 to 68.34
B0	C	NUPM	36.00	-9.83 to 100.52
B0	C	GW	57.88	26.32 to 122.44
B0	C	SWC	4.05	-2.73 to 12.97
B0	C	PostLAI _m	38.38	-11.14 to 100.48
B0	C	PostSPAD _m	12.85	-12.03 to 43.80
B0	S	DMA	41.71	3.24 to 98.22
B0	S	NUPA	40.57	-1.46 to 97.36
B0	S	PostNUP	30.38	-6.46 to 89.29
B0	S	NUPM	47.37	0.02 to 117.39
B0	S	GW	70.28	36.46 to 132.88
B0	S	SWC	12.48	3.19 to 30.22
B0	S	PostLAI _m	51.06	-2.60 to 129.77
B0	S	PostSPAD _m	23.62	-6.14 to 62.82
B20	O	DMM	138.49	43.37 to 380.50
B20	O	HI	26.40	4.69 to 77.65
B20	O	PostDM	111.50	31.16 to 276.96
B20	O	DMA	46.70	7.53 to 128.02
B20	O	DMT	3.65	-1.66 to 16.70
B20	O	NUPA	77.46	17.45 to 214.09
B20	O	PostNUP	50.78	15.13 to 120.19
B20	O	NUPM	90.25	24.77 to 227.99
B20	O	GW	7.09	-1.55 to 20.24
B20	O	GN	159.45	38.79 to 451.88

Group	Model	Trait	Mean <i>MSE</i> increase (%)	95% bootstrap CI (%)
B20	O	SWC	1.40	-3.27 to 8.94
B20	O	PostLAI _m	59.92	21.22 to 143.55
B20	O	PostSPAD _m	74.99	14.17 to 206.66
B20	C	DMM	156.77	57.79 to 338.11
B20	C	DMA	51.76	7.75 to 123.34
B20	C	NUPA	91.09	24.49 to 216.05
B20	C	PostNUP	60.05	20.50 to 138.26
B20	C	NUPM	107.76	35.16 to 249.61
B20	C	GW	9.92	-2.24 to 26.57
B20	C	SWC	0.54	-7.47 to 8.48
B20	C	PostLAI _m	75.90	35.44 to 173.70
B20	C	PostSPAD _m	93.26	29.00 to 233.19
B20	S	DMA	70.97	23.02 to 176.61
B20	S	NUPA	105.28	41.69 to 254.29
B20	S	PostNUP	79.86	33.06 to 173.85
B20	S	NUPM	117.74	50.66 to 260.46
B20	S	GW	20.09	-0.42 to 53.60
B20	S	SWC	3.77	-4.15 to 11.68
B20	S	PostLAI _m	97.91	51.45 to 201.66
B20	S	PostSPAD _m	116.37	46.61 to 286.08

Model codes: O, original; C, core exclusion; S, strict exclusion. All 60 trait model predictor records are shown. The N rate baseline is reported separately in [Table S1](#).

Mean values and intervals come from the same omitted original block bootstrap procedure, rather than combining LOBO point estimates with bootstrap intervals. Each draw samples four whole blocks with replacement within each season. Importance is calculated by within block trait permutation and scored only on omitted original blocks. Of 500 draws, 494 were evaluable; six omitted no block and were skipped, with no model fitting failure.

Percentage = $100 \times \text{signed increase in held out } MSE / \text{baseline held out } MSE$. It is not a yield contribution percentage or relative importance summing to 100%. Intervals are the 2.5th and 97.5th percentiles; negative estimates are retained. Different zero crossing patterns between biochar groups do not establish a significant group difference.

Table S4 PSEM model fit and influence diagnostics

Panel A Yield component model fit

Group	Structure	Yield R^2_m (95% CI)	Yield R^2_c (95% CI)	Fisher C	df	P
B0	Original	0.962 (0.952 to 0.979)	0.962 (0.953 to 0.979)	13.507	14	0.487
B0	GN removed	0.932 (0.922 to 0.957)	0.932 (0.923 to 0.958)	8.941	8	0.347
B0	Strict	0.927 (0.914 to 0.956)	0.927 (0.914 to 0.956)	11.770	8	0.162
B20	Original	0.980 (0.979 to 0.988)	0.980 (0.979 to 0.988)	5.462	14	0.978
B20	GN removed	0.957 (0.949 to 0.976)	0.959 (0.949 to 0.977)	1.308	8	0.995
B20	Strict	0.953 (0.939 to 0.975)	0.957 (0.942 to 0.977)	1.623	8	0.990

Panel B Collinearity and leave block global fit

Group	Structure	Maximum Yield VIF	Minimum Fisher P	Maximum Fisher P	Fits with $P < 0.05$
B0	Original	60.46	0.211	0.844	0/8
B0	GN removed	17.50	0.118	0.970	0/8
B0	Strict	15.57	0.041	0.911	2/8
B20	Original	88.57	0.757	0.992	0/8
B20	GN removed	42.48	0.651	0.998	0/8
B20	Strict	17.11	0.681	0.998	0/8

Original PSEM contains NUPA, PostNUP, DMA, GN, PostDM and Yield response nodes. GN removed excludes GN and all its attached paths. Strict excludes GN and PostDM and all their attached paths. No replacement paths are added. Nc and Nc², Season and a season by block random intercept are retained.

R^2_m and R^2_c are fitted mixed model quantities, not out of sample predictive R^2 . Intervals use 1000 whole block bootstrap refits stratified by season; all requested component sets fitted successfully. $P > 0.05$ for Fisher C does not verify mechanism or causality. Summed component AIC must not be compared across different response node sets.

Leave block results omit each of the eight blocks once and measure influence, not predictive validation. Maximum VIF is taken from the Yield fixed effect equation. The strict model's high R^2 with retained N terms does not validate removed GN or PostDM pathways. Only four independent blocks are available per season.

Table S5 PostDM association with Yield before and after GN exclusion

Group	Structure	β	Model P	95% bootstrap CI	Leave block β range	Fits with $P < 0.05$
B0	Original	0.270	0.005	0.143 to 0.428	0.222 to 0.314	8/8
B0	GN removed	0.251	0.043	0.058 to 0.496	0.193 to 0.330	4/8
B20	Original	0.286	0.001	0.052 to 0.460	0.200 to 0.382	8/8
B20	GN removed	0.263	0.033	0.008 to 0.546	0.116 to 0.365	5/8

All coefficients use the full biochar group means and SDs held fixed across sensitivity refits. Each coefficient has 1000 valid bootstrap refits and eight valid leave block refits. There are no leave block sign reversals for these four paths. Model P values and percentile intervals use different inferential procedures and need not agree at 0.05.

Positive coefficients and intervals after GN exclusion support persistence of a conditional association. They do not eliminate PostDM's biomass balance dependence or independently establish an assimilate flux mechanism.

Table S6 Yield predictors across the three PSEM structures

Group	Model	Predictor	β	Model <i>P</i>	95% bootstrap CI	Leave block β range	Sign reversals
B0	O	Nc	-0.665	0.002	-1.076 to -0.177	-0.745 to -0.487	0/8
B0	O	Nc ²	-0.239	0.012	-0.410 to -0.094	-0.290 to -0.192	0/8
B0	O	DMA	-0.112	0.290	-0.361 to 0.141	-0.181 to -0.029	0/8
B0	O	GN	1.296	<0.001	0.812 to 1.675	1.121 to 1.403	0/8
B0	O	PostDM	0.270	0.005	0.143 to 0.428	0.222 to 0.314	0/8
B0	G	Nc	0.470	0.002	0.053 to 0.809	0.350 to 0.582	0/8
B0	G	Nc ²	-0.510	<0.001	-0.696 to -0.277	-0.568 to -0.438	0/8
B0	G	DMA	0.023	0.869	-0.263 to 0.399	-0.096 to 0.119	3/8
B0	G	PostDM	0.251	0.043	0.058 to 0.496	0.193 to 0.330	0/8
B0	S	Nc	0.606	<0.001	0.218 to 0.911	0.523 to 0.726	0/8
B0	S	Nc ²	-0.703	<0.001	-0.821 to -0.542	-0.751 to -0.639	0/8
B0	S	DMA	0.022	0.876	-0.266 to 0.411	-0.084 to 0.112	3/8
B20	O	Nc	-0.584	0.002	-0.931 to -0.001	-0.765 to -0.261	0/8
B20	O	Nc ²	-0.007	0.922	-0.227 to 0.133	-0.125 to 0.065	4/8
B20	O	DMA	0.147	0.087	-0.061 to 0.327	0.038 to 0.205	0/8
B20	O	GN	1.116	<0.001	0.715 to 1.432	0.942 to 1.212	0/8
B20	O	PostDM	0.286	0.001	0.052 to 0.460	0.200 to 0.382	0/8
B20	G	Nc	0.490	0.008	0.058 to 0.876	0.364 to 0.742	0/8
B20	G	Nc ²	-0.246	0.007	-0.437 to -0.030	-0.381 to -0.192	0/8
B20	G	DMA	0.173	0.163	-0.082 to 0.481	0.002 to 0.254	0/8
B20	G	PostDM	0.263	0.033	0.008 to 0.546	0.116 to 0.365	0/8
B20	S	Nc	0.813	<0.001	0.606 to 0.952	0.749 to 0.886	0/8
B20	S	Nc ²	-0.413	<0.001	-0.496 to -0.306	-0.455 to -0.380	0/8
B20	S	DMA	0.055	0.635	-0.133 to 0.310	-0.054 to 0.134	1/8

PSEM codes: O, original; G, GN removed; S, strict. All 24 prespecified standardized Yield predictors are shown; intercept and Season are omitted as adjustment terms. Nc = NR – 175 and Nc² = (NR – 175)², with both terms standardized. Each row has 1000 valid bootstrap refits and eight valid leave block refits. Sign reversal counts compare leave block coefficient direction with the full model coefficient.

Values are model conditional associations, and the GN coefficients contain mathematical coupling. Strict PSEM retains the PostNUP response equation but contains no directed PostNUP to Yield path after GN and PostDM removal; that absence is a model specification, not evidence of biological absence.