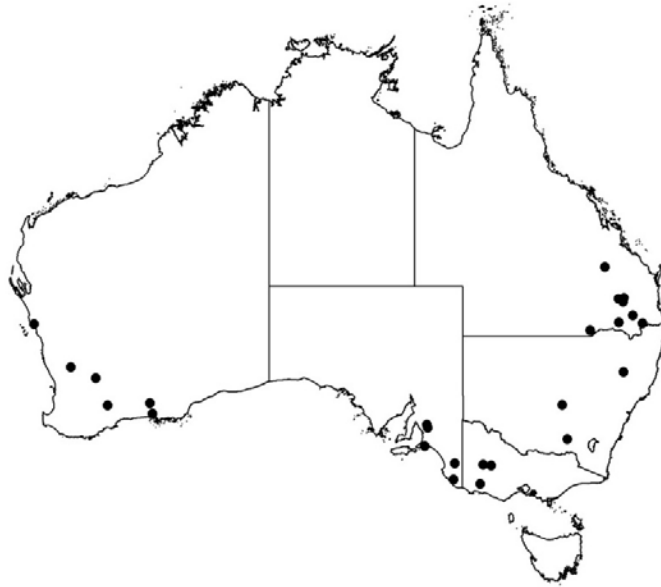Biogeosciences

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Supplement of

Convergent modelling of past soil organic carbon stocks but divergent projections

Z. Luo et al.

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Supplement Figure S1. The geographical distribution of the 28 experimental sites where data are used in this study. See Table 1 in the supplement for details of the management and climate conditions at these sites.
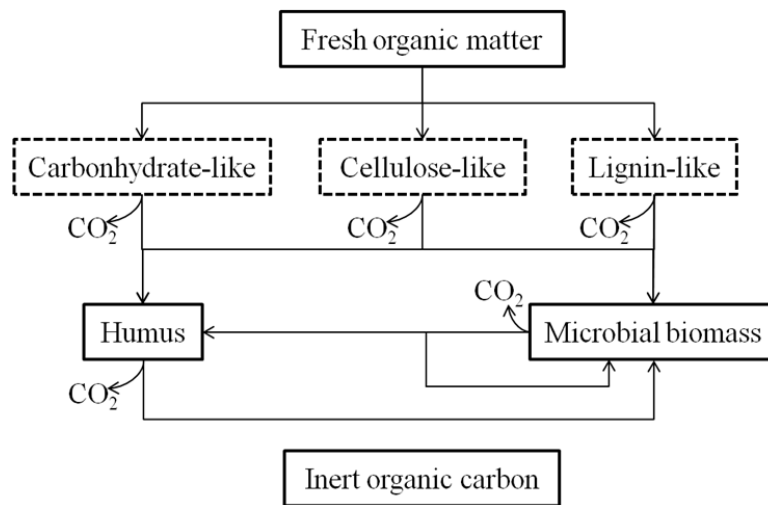
Supplement Figure S2. The transformation of soil organic carbon (SOC) pools in APSIM.
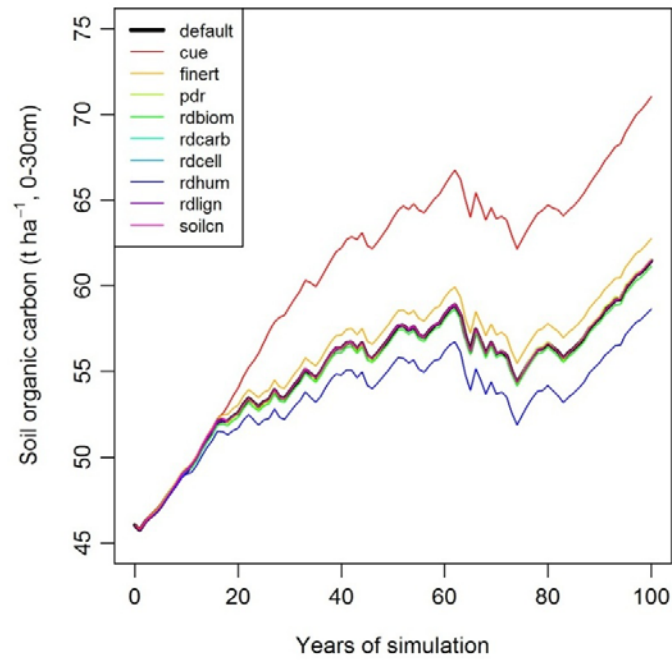
Supplement Figure S3. Sensitivity of modeled soil organic carbon to different model parameters. Simulated soil organic carbon dynamics under a 10% increase of a parameter value (color lines) is compared with that using default value (black bold line) under a continuous wheat system. See Table 2 in the supplement for the meaning of the legends.
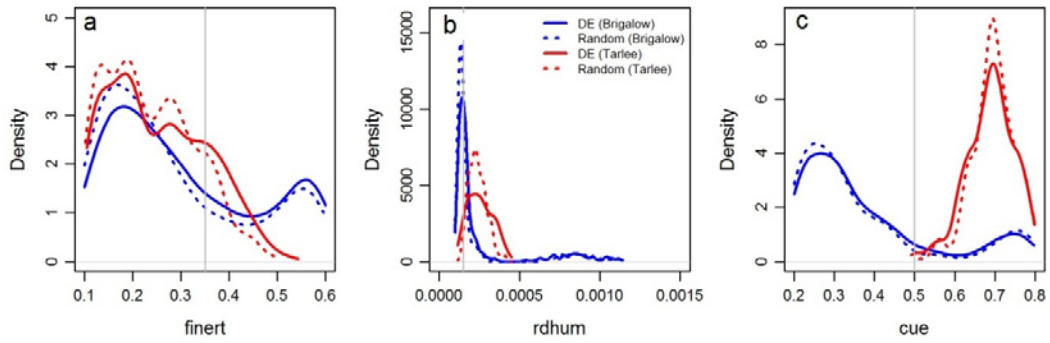
Supplement Figure S4. Posterior distributions of the three most important parameters at Brigalow and Tarlee of Australia. a, finert – fraction of inert organic carbon in total soil organic carbon. b, rdhum – potential decomposition rate of humic organic carbon. c, *CUE* – microbial carbon use efficiency. The distribution derived using the differential evolution optimization (DE) are compared with that derived using the random sampling (Random) approach. Grey vertical lines show the default values of the three parameters in the model. See more details in the Methods section for the two optimization approaches. See Fig. 2c and d for the relationship of the three parameters at Tarlee and Brigalow respectively.
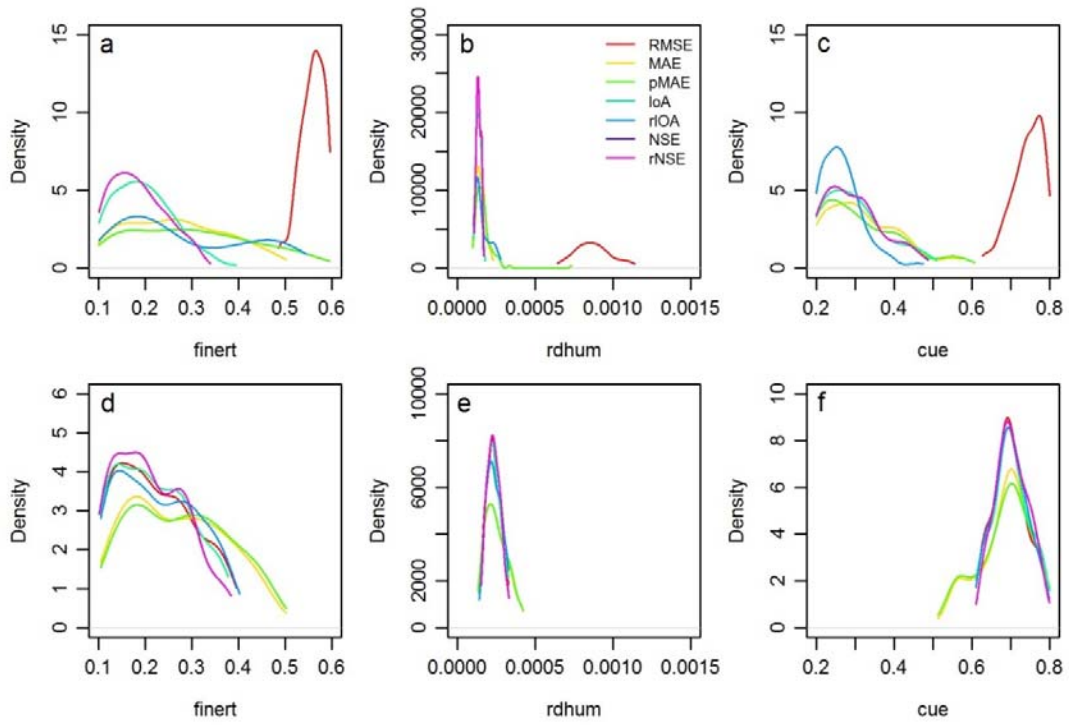
Supplement Figure S5. The effect of selection criterions on the optimized posterior distributions of model parameters (finert, rdhum and *CUE*) at Brigalow (a, b and c) and Tarlee (d, e and f) of Australia. See Table 3 in the supplement for the seven criteria showed in the legend.

Supplement Table S1. Climate conditions and management of the studied experiments in Australia. Data adopted from Skjemstad and Spouncer (2003).

Location	Rainfall (mm)	Temperature (°C)	Management[*]
Brigalow, Qld	686	21.1	W/S–R–Z–0–3–18
Warra Field Trial, Qld	655	19.2	W/F–R–C–0–1–13
			W/P/F–R–C–75–1–13
			W/F–R–C–75–1–13
Hermitage, Qld	649	16.4	W–B–C–50–1–19
			W–B–Z–50–1–19
			W–R–C–50–1–19
Langlands–Logie, Qld	655	19.7	W–R–Z–0–1–46
			W/S–R–Z–0–1–21
Warra, Qld	660	19.3	W/S–R–0–1–66
			W/P–R–0–1–66
Cecilvale, Qld	655	19.6	W/F–R–0–1–36
			W–R–0–1–6
			W/S–R–0–1–9
Waco, Qld	655	19.6	W/S/F–R–0–1–70
			W–R–0–2–2
			W/S–R–0–1–19
Thallon, Qld	499	20.4	W–R–0–1–4
			W/S–R–0–1–20
Billa Billa, Qld	585	19.3	W/S–R–0–2–(25, 20)
			W/P–R–0–1–20
Condobolin, NSW	427	17.6	W–B–Z–0–1–15
Tamworth, NSW	665	17.2	W/S/F–R–Z–0–2–30
			W/S/P–R–Z–0–2–30

Wagga Wagga, NSW	522	16.0	W–R–Z–0–1–12
Hamilton, Vic	692	13.0	P–R–Z–0–3–17
Horsham, Vic	439	14.8	W/F–R–Z–0–2–83
			W/F/P–R–Z–0–2–83
Glenorchy, Vic	426	14.6	W/O/P/F–R–Z–0–1–23
Tarlee, SA	462	16.9	W–R–Z–0–1–18
			W/S–R–Z–0–1–18
			W/F–R–Z–0–1–18
			W/P–R–Z–0–1–18
Freeling, SA	463	15.9	B/P–R–Z–0–1–27
Padthaway, SA	517	14.8	W/P–R–Z–0–1–24
Glencoe, SA	770	13.8	P–R–Z–0–1–24
Chapman, WA	457	19.6	W–R–Z–0–1–23
			P–R–Z–0–1–23
			W/P1–R–Z–0–1–23
			W/P2–R–Z–0–1–23
			W/P3–R–Z–0–1–23
East Beverley, WA	369	18.2	W–R–Z–0–1–7
			P–R–Z–0–1–7
			W/P1–R–Z–0–1–7
			W/P2–R–Z–0–7
			W/P3–R–Z–0–1–7
Gibson, WA	517	16.0	W–R–Z–0–1–18
			P–R–Z–0–1–18
			P/W/L1–R–Z–0–1–18
			P/W/L2–R–Z–0–1–18

Merredin (heavy), WA	333	17.8	W–R–Z–0–1–18
			P–R–Z–0–1–18
			W/P1–R–Z–0–1–18
			W/P2–R–Z–0–1–18
			W/P3–R–Z–0–1–18
			W/P4–R–Z–0–1–18
Merredin (light) , WA	333	17.8	W–R–Z–0–1–11
			W/P1–R–Z–0–1–11
			W/P2–R–Z–0–1–11
			W/P3–R–Z–0–1–11
			W–R–C–0–1–11
			W/P1–R–C–0–1–11
			W/P2–R–C–0–1–11
			W/P3–R–C–0–1–11
Newdegate, WA	356	16.2	W–R–Z–0–1–21
			P–R–Z–0–1–21
			W/P1–R–Z–0–1–21
			W/P2–R–Z–0–1–21
			W/P3–R–Z–0–1–21
Salmon Gums, WA	352	16.0	W–R–C–0–1–14
			W/P1–R–C–0–1–14
			W/P2–R–C–0–1–14
Wongan Hills, WA	370	18.2	W/P1–R–C–0–2–6
			W/P2–R–C–0–2–6

[*] Rotation (i.e., W/S)–Residue (B for burned or removed, R for retained)–Tillage (C for conventional tillage, Z for no-till)–Fertilizer (e.g., 50 for 50 kg N ha^{-1} yr^{-1})–Soil types (e.g., 2 for the experiment was conducted under two soil types)–Experimental duration (e.g., 10 for 10 years). B, barely; W, wheat; O, oats; S, sorghum; P, pasture; F, fallow; L, lupin.

Supplement Table S2. Model parameters analyzed for the sensitivity analysis in the study.

Parameter (unit)[*]	Default value used for sensitivity analysis	Importance index	Prior distribution [min, max]
CUE (unitless)	0.5	64.43	[0.2, 0.8]
finert (unitless)	0.35	8.93	[0.1, 0.6]
k_{surfc} (day^{-1})	0.1	0.96	–
k_{biom} (day^{-1})	0.0081	2.23	–
k_{carb} (day^{-1})	0.2	0.012	–
k_{cell} (day^{-1})	0.05	0.088	–
k_{lign} (day^{-1})	0.0095	0.0097	–
k_{hum} (day^{-1})	0.00015	18.79	[0.000015, 0.0015]
soilcn (unitless)	12	0.50	–

[*]*CUE*: microbial carbon use efficiency (unitless); finert: initial fraction of inert organic matter in total SOC (unitless); k_{surfc}: potential decomposition rate for aboveground FOM (day^{-1}); k_{biom}: potential decomposition rate for microbial biomass; k_{carb}: potential decomposition rate for carbohydrate–like C in belowground FOM; k_{cell}: potential decomposition rate for cellulose–like C in belowground FOM; k_{lign}: potential decomposition rate for lignin–like C in belowground FOM; k_{hum}: potential decomposition rate for humic organic matter; soilcn: carbon to nitrogen ratio of soil.

Supplement Table S3. Performance measures for comparing model predictions and observations.

Criterion	Formulation[*]	Range[†]
Root mean square error (RMSE)	$\sqrt{\dfrac{\sum_{i=1}^{N}(P_i - O_i)^2}{N}}$	[**0**, $+\infty$]
Mean absolute error (MAE)	$\dfrac{\sum_{i=1}^{N}|P_i - O_i|}{N}$	[**0**, $+\infty$]
Percentage MAE (pMAE)	$\dfrac{\sum_{i=1}^{N}\left|\dfrac{P_i - O_i}{O_i}\right|}{N}$	[**0**, $+\infty$]
Index of agreement (IoA)	$\dfrac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}(|P_i - \bar{P}| + |O_i - \bar{O}|)^2}$	[**1**, $+\infty$]
Relative IoA (rIoA)	$\dfrac{\sum_{i=1}^{N}\left(\dfrac{P_i - O_i}{O_i}\right)^2}{\sum_{i=1}^{N}\left(\dfrac{|P_i - \bar{P}| + |O_i - \bar{O}|}{\bar{O}}\right)^2}$	[**1**, $+\infty$]
Nash–Sutcliffe Efficiency (NSE)	$\dfrac{\sum_{i=1}^{N}(P_i - O_i)^2}{\sum_{i=1}^{N}(P_i - \bar{O})^2}$	[**1**, $+\infty$]
Relative NSE (rNSE)	$\dfrac{\sum_{i=1}^{N}\left(\dfrac{P_i - O_i}{O_i}\right)^2}{\sum_{i=1}^{N}\left(\dfrac{P_i - \bar{O}}{\bar{O}}\right)^2}$	[**1**, $+\infty$]

[*]P_i and O_i denote the predicted and observed value i; $\bar{O}$ is the mean of observed values.
[†]The bold number shows the target value when reach perfect match, i.e., no difference between predicted and observed values.