

Assessing Thermodynamic Parameter Sensitivity for Simulating Temperature Response of Soil Nitrification

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Electronic supplementary information

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Introduction

Supplementary information contains 3 tables with basic information on edaphic properties of selected soils, unknown parameter fitting results for SQRT and MMRT models (S1) and ANOVA analysis to compare significant difference between models' performances and estimated parameter values for different temperature ranges (S2). Moreover, figure S1, S2, S3 and S4 demonstrate soil sampling sites across Taiwan, step-by-step procedure for global sensitivity analysis, scatter plot of parameter sensitivity analysis for square root growth model (SQRT) and macromolecular rate theory model (MMRT) and variation in optimum temperature (T_{opt}) for nitrification among soils at different temperature ranges, respectively.

Supplementary material

Table S1. Edaphic properties of selected soil plots.

	Land Cover Type	Description	Mean annual temperature C°	pH	TOC g/kg	TN g/kg
Miaoli County, Taiwan	FR1	Forest soil	23.12	5.03	18.64	1.25
	FR2	Forest soil		5.63	12.68	1.24
	FL1	Fallow land		6.35	17.20	1.40
	FL2	Fallow land		6.42	8.83	0.97
	CL2	Cropped		5.58	12.27	1.30
	CL6	Cropped		6.45	14.32	1.47
Kaohsiung County, Taiwan	FR3	Forest soil	25.85	7.01	11.78	0.80
	FL3	Fallow land		6.50	17.40	3.15
	CL1	Cropped		6.70	23.81	2.88
Taoyuan city, Taiwan	FL4	Fallow land	23.24	6.2	12.18	0.97
	FR4	Forest soil		6.02	11.91	2.08
	CL3	Cropped		6.17	10.04	1.53
Pingtung city, Taiwan	FL5	Fallow land	24.96	6.61	15.08	1.69
	CL5	Cropped		7.21	10.02	0.94
Chiayi County, Taiwan	FL6	Fallow land	24.22	6.23	8.43	1.12
	CL4	Cropped		5.65	13.11	1.80

TOC: Total organic carbon, TN: Total nitrogen

Table S2. Unknown parameters estimated by SQRT and MMRT models and their accuracy in simulating nitrification response to temperature. (FR: forest soil, FL: fallow land, CL: cropping land). Note; a variation of ± 0.015 for likelihood functions (NSE and r) may be possible while replicating of these results since sensitive parameters such as T_{\max} , $\Delta S_{T_o}^{\ddagger}$ and a are rounded up from more than five decimal digits to two to three decimal digits.

Temperature range	Land Cover Type	SQRT						MMRT						
		a	b	T_{\min}	T_{\max}	T_{opt}	NSE*	r^{**}	$\Delta H_{T_o}^{\ddagger}$	$-(\Delta C_p^{\ddagger})$	$-(\Delta S_{T_o}^{\ddagger})$	T_{opt}	NSE*	r^{**}
				°C	°C	°C							°C	
4 to 40°C	FR1	0.043	0.398	-4.81	42.82	35.64	0.88	0.94	32.14	5.30	0.137	31.50	0.89	0.95
	FR2	0.051	0.396	-2.96	42.93	35.83	0.92	0.97	45.11	3.63	0.093	37.80	0.88	0.94
	FR3	0.084	0.108	-1.98	43.50	29.71	0.81	0.90	10.14	10.89	0.21	26.30	0.85	0.93
	FL1	0.034	0.574	-2.71	42.10	36.53	0.95	0.98	34.84	3.59	0.133	35.10	0.90	0.96
	FL2	0.031	0.571	-3.61	41.86	36.33	0.92	0.97	45.42	6.47	0.101	32.40	0.87	0.94
	FL3	0.032	0.326	-15.37	41.55	32.82	0.83	0.91	7.94	10.83	0.225	26.10	0.84	0.92
	CL1	0.077	0.502	-3.29	41.45	35.41	0.88	0.94	31.10	7.87	0.135	29.30	0.88	0.94
	CL2	0.026	0.649	-4.56	41.88	36.76	0.93	0.97	38.15	4.77	0.126	33.30	0.92	0.96
20 to 45°C	FR4	0.108	0.044	-2.99	51.83	32.76	0.80	0.92	52.80	8.84	0.066	31.32	0.89	0.94
	FL4	0.112	0.041	-1.61	52.00	32.16	0.87	0.94	41.36	7.54	0.103	30.84	0.93	0.97
	FL5	0.039	0.035	-2.70	49.09	29.92	0.84	0.92	48.66	13.45	0.106	28.97	0.95	0.98
	FL6	0.089	0.048	-4.50	50.00	32.26	0.96	0.98	24.38	7.59	0.161	28.56	0.97	0.99
	CL3	0.038	0.043	-1.36	50.34	31.18	0.84	0.92	44.80	8.27	0.112	30.77	0.88	0.96
	CL4	0.064	0.043	-1.22	48.77	30.03	0.85	0.94	42.82	10.16	0.111	29.56	0.94	0.98
	CL5	0.084	0.048	-1.56	45.60	28.40	0.91	0.95	23.70	11.59	0.172	27.40	0.96	0.99
	CL6	0.099	0.043	-0.57	50.22	30.82	0.90	0.95	58.07	10.28	0.054	30.99	0.98	0.99

Note: * Nash-Sutcliffe Coefficient; ** Correlation Constant; T_{\min} : Minimum temperature; T_{\max} : Maximum temperature; T_{opt} : Optimum temperature; $\Delta H_{T_o}^{\ddagger}$: Change of enthalpy; $\Delta S_{T_o}^{\ddagger}$: Change of entropy; ΔC_p^{\ddagger} : Change in heat capacity.

Table S3. ANOVA analysis to compare significant difference between models' performances and estimated parameter values for different temperature ranges (similar data for remaining parameters are not shown here).

	<i>F</i>	<i>P-value</i>
ANOVA analysis to compare significant difference in NSE coefficient between SQRT simulated and observed NP rates over temperature ranges (4 °C to 40°C and 20 °C to 45 °C).	13.2036	**
ANOVA analysis to compare significant difference in NSE coefficient between MMRT simulated and observed NP rates over temperature ranges (4 °C to 40°C and 20 °C to 45 °C).	0.5643	0.4650
ANOVA analysis to compare significant difference between T_{\min} estimated for different temperature ranges (4 °C to 40°C and 20 °C to 45 °C).	3.19	0.096
ANOVA analysis to compare significant difference between T_{\max} estimated for different temperature ranges (4 °C to 40°C and 20 °C to 45 °C).	96.3676	**
ANOVA analysis to compare significant difference ΔC_p^{\ddagger} estimated for different temperature ranges (4 °C to 40°C and 20 °C to 45 °C).	5.7173	*
Note: *: p-value<0.05; **: p-value<0.01		

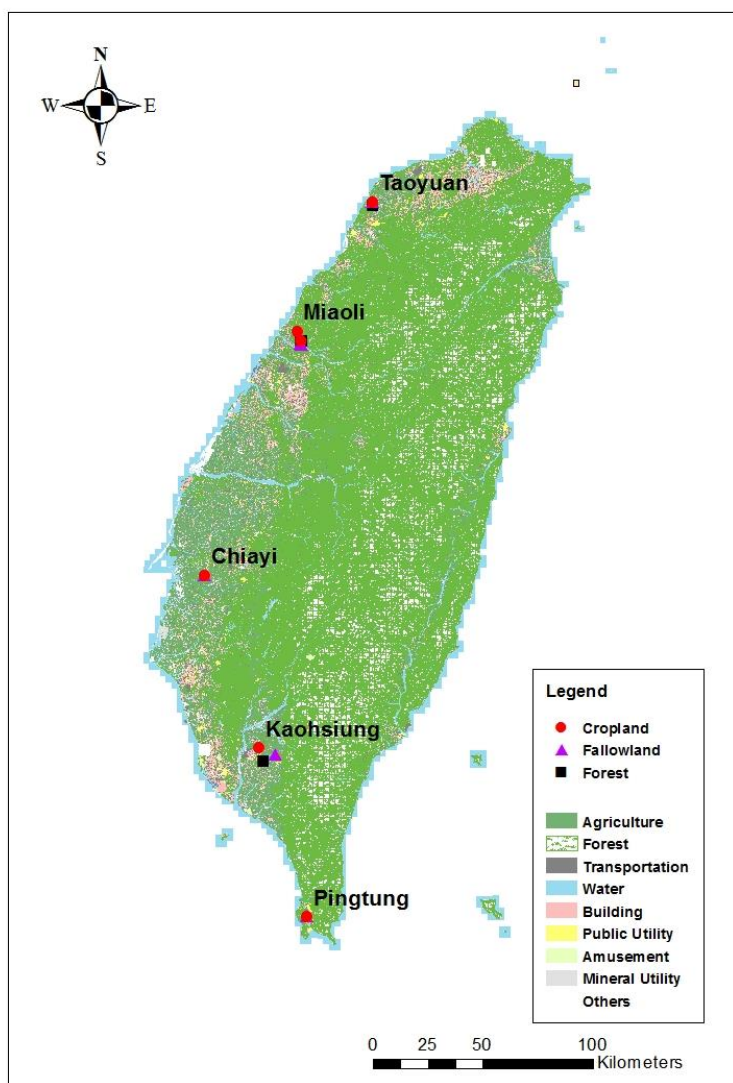


Figure S1. Map representing the soil sampling sites across Taiwan.

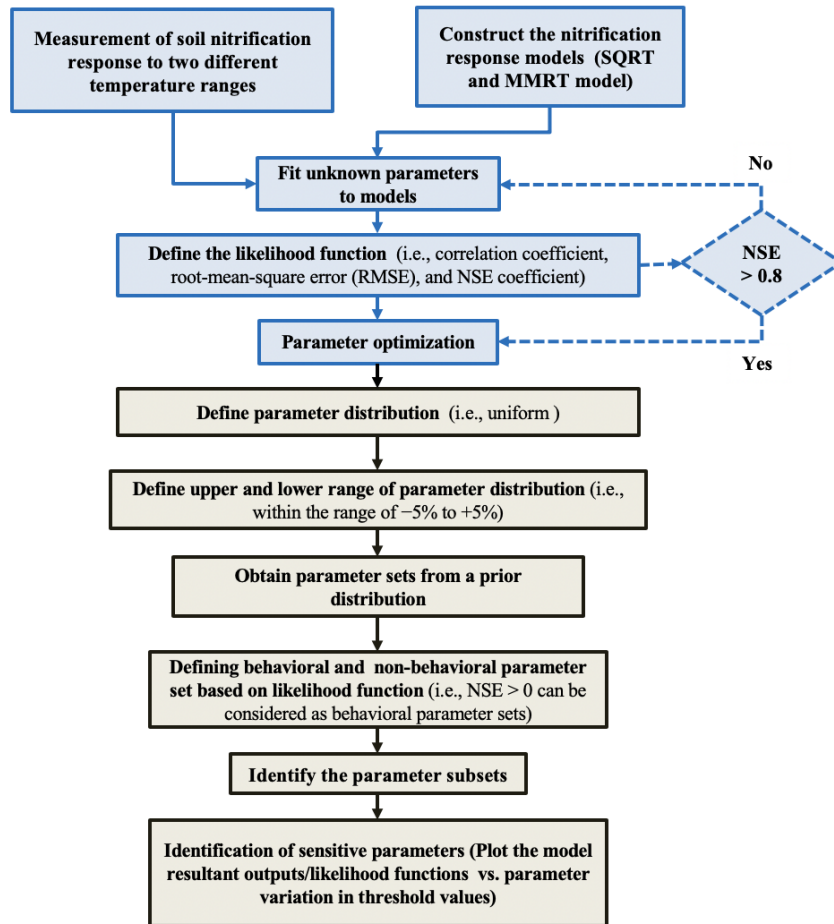


Figure S2. A step-by-step procedure for global sensitivity analysis which was used in this study.

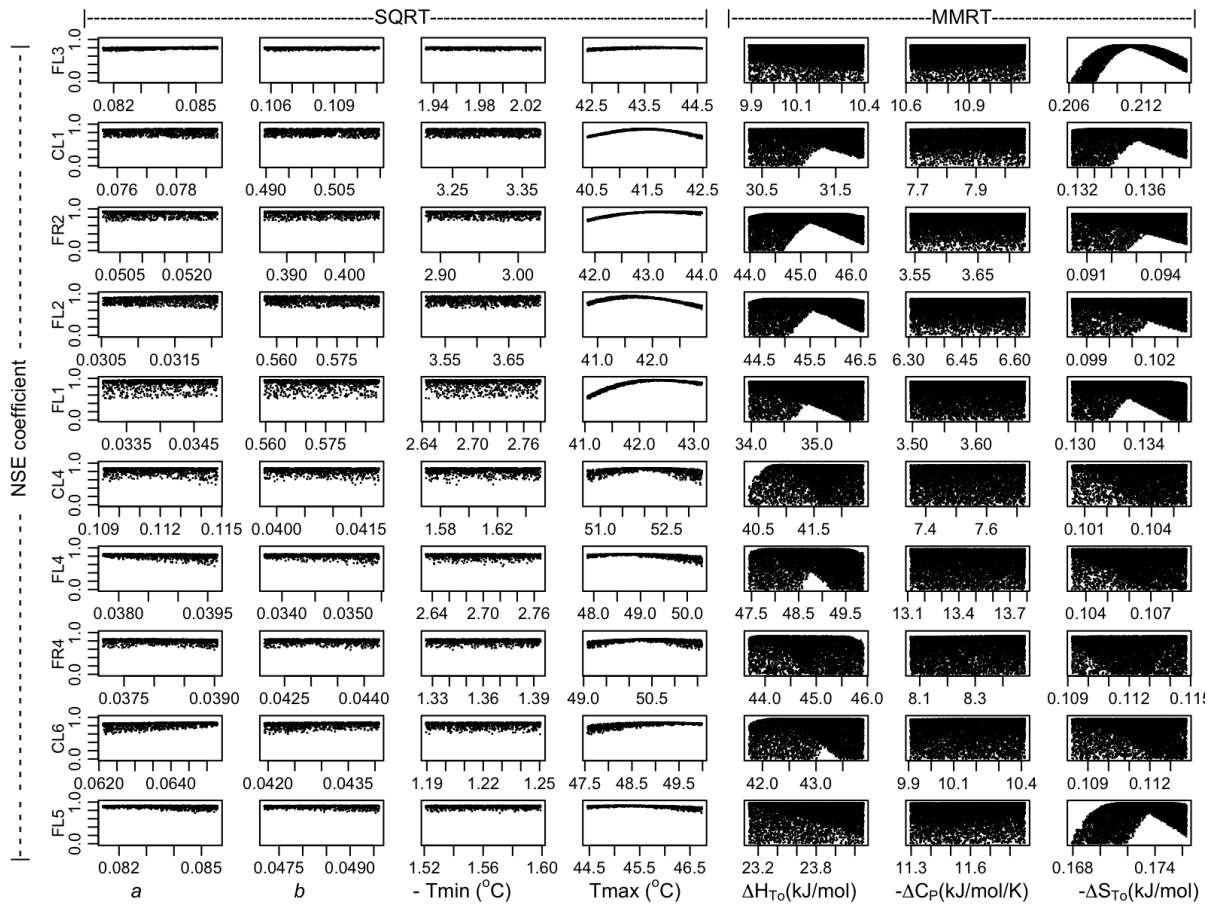


Figure S3. Scatter plot of parameter sensitivity analysis for square root growth model (SQRT) and macromolecular rate theory model (MMRT). FR, FL, and CL represent soil samples from forest land, fallow land, and cropland, respectively. From top, rows 1-5 indicate parameter sensitivity for soils incubated between 4°C and 40°C, rows 6-10 indicate parameter sensitivity for soils incubated between 20°C and 45°C.

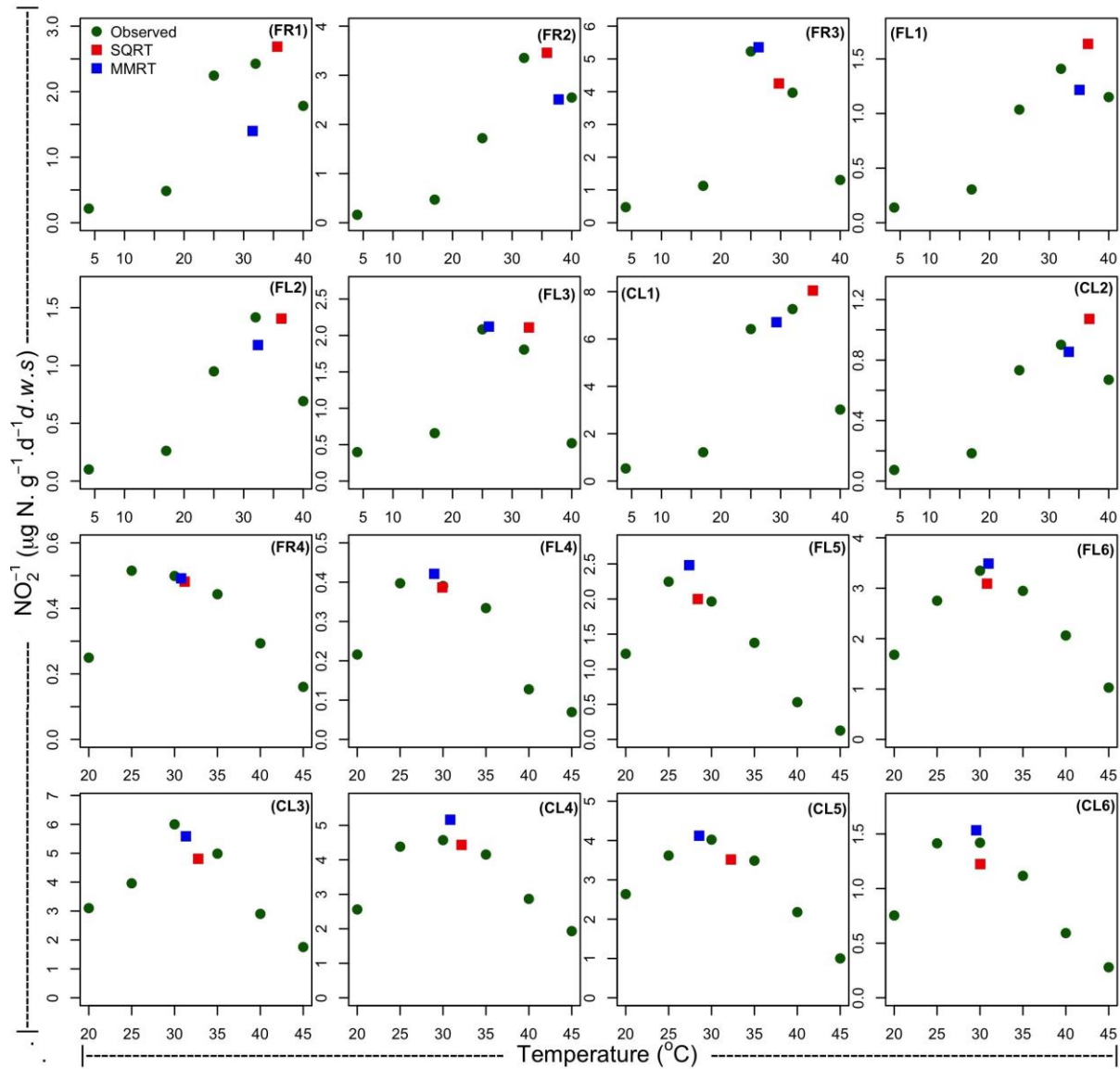


Figure S4. Variation in T_{opt} and associated nitrification, estimated by SQRT and MMRT model (red and blue points, respectively) and observed nitrification (dark green points) among soils at different temperature ranges. FR, FL, and CL represent soil samples from forest land, fallow land, and cropland, respectively.