

Supplementary data

Sorption–desorption of dimethoate in urban soils and potential environmental impacts

**Islam Md Meftaul,^{a,b} Kadiyala Venkateswarlu,^c Rajarathnam Dharmarajan,^a
Prasath Annamalai,^a and Mallavarapu Megharaj^{*,a, d}**

^aGlobal Centre for Environmental Remediation (GCER), Faculty of Science, The University of Newcastle, Callaghan, NSW 2308, Australia

^bDepartment of Agricultural Chemistry, Sher-e-Bangla Agricultural University, Dhaka-1207, Bangladesh

^cFormerly Department of Microbiology, Sri Krishnadevaraya University, Anantapuramu 515003, India

^dCooperative Research Centre for Contamination Assessment and Remediation of the Environment (CRC CARE), The University of Newcastle, Callaghan, NSW 2308

**Address for correspondence:*

Prof. Mallavarapu Megharaj

Global Centre for Environmental Remediation (GCER)

Faculty of Science

The University of Newcastle, ATC Building

University Drive, Callaghan, NSW 2308, Australia

Mobile: +61 2 49138734; orcid.org/0000-0002-6230-518X

E-mail: megh.mallavarapu@newcastle.edu.au

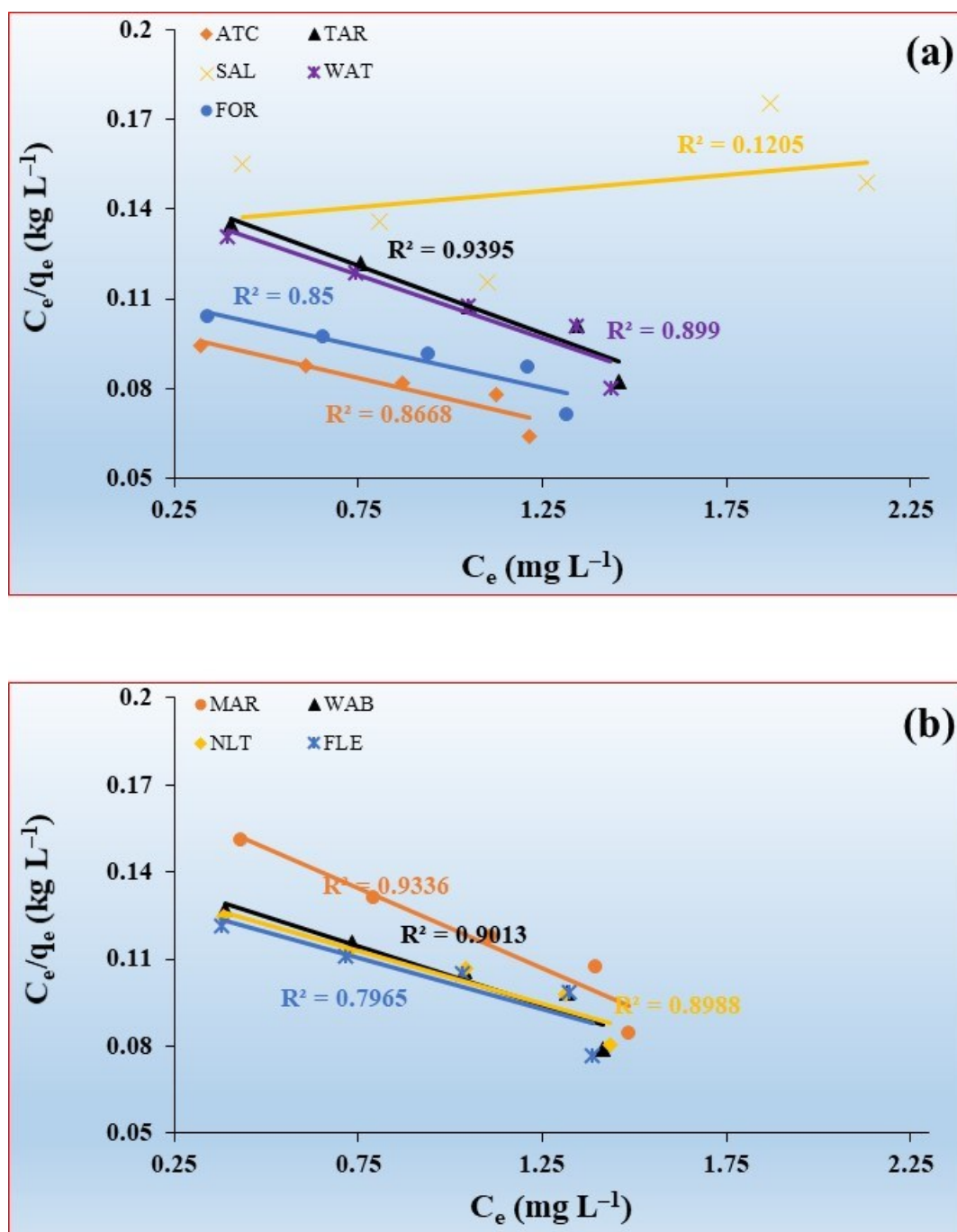


Figure S1. Langmuir sorption isotherms for (a, b) dimethoate in nine different urban soils.

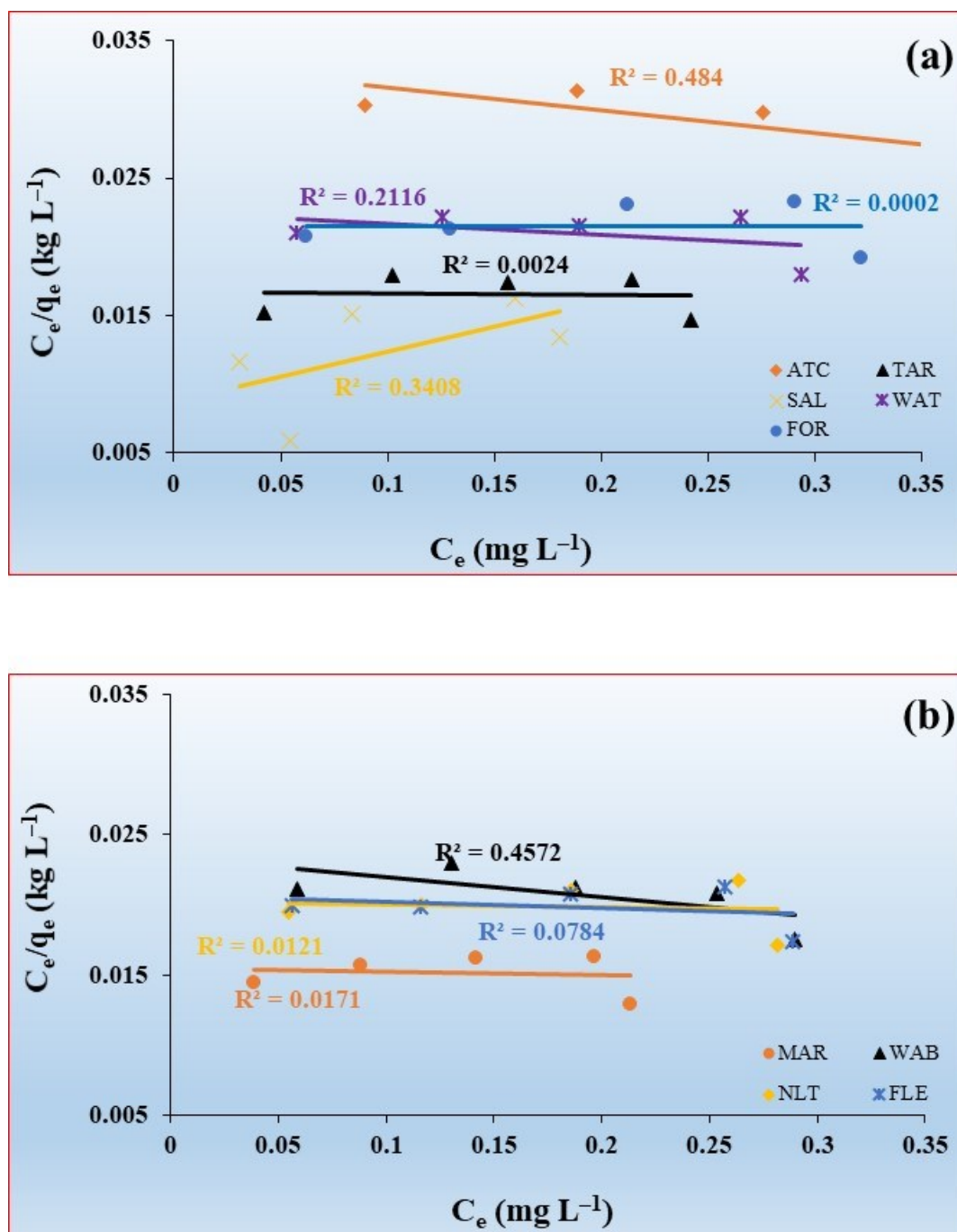


Figure S2. Langmuir desorption isotherms for (a, b) dimethoate in nine different urban soils.

Table S1. Physico-chemical properties of urban soils collected in and around Newcastle, Australia.

Location	Soil collection area	Soil ID	pH (in Milli-Q water)	Major mineral compound	TOC (%)	Fe (%)	Al (%)	Clay (%)	Silt (%)	Sand (%)	Textural class
Home garden	Taree	TAR	7.5 ± 0.03	Quartz, Sinnerite, Ice Ic, Sylvine, Bernalite, Albite	2.02 ± 0.01	1.19± 0.03	0.92±0.11	11.2	55	33.8	Silt loam
	Fletcher	FLE	6.6 ± 0.03	Quartz, Oligoclase, Albite, Sodalite	1.29 ±0.02	0.03±0.67	0.01±0.99	12.4	23.8	63.8	Sandy loam
	Salamander Bay	SAL	6.1 ± 0.02	Quartz, Dolomite, Zeolite LC-3, Palladium	0.25 ±0.16	1.42±0.02	0.65±0.15	1.2	1.2	97.6	Sand
Lawn	UoN-1	ATC	5.8 ± 0.03	Quartz, Orthoclase, Albite, Hyalophane	7.66 ±0.01	1.10±0.09	0.73±0.11	7.5	41.2	51.3	Loam
	UoN-2	FOR	6.2 ± 0.05	Quartz, Marshite, Albite, Zeolite	3.52 ±0.01	1.95±0.05	1.27±0.13	7.4	23.8	68.8	Sandy loam
	Warabrook	WAB	6.6 ± 0.04	Quartz, Birnessite, Albite, Sinnerite	1.44 ±0.04	1.40±0.21	0.96±0.11	18.7	25	56.3	Sandy loam
Park	Maryland	MAR	8.0 ± 0.01	Quartz, Albite, Zeolite, Sodalite	0.21 ±0.10	3.15±0.03	0.73±0.18	7.5	16.2	76.3	Loamy sand
	Waratah	WAT	5.8 ± 0.03	Quartz, Birnessite, Zeolite Rho, Albite	0.19 ±0.21	1.08±0.06	0.81±0.14	30.0	41.2	28.8	Loam
	Lambton	NLT	5.5 ± 0.05	Quartz, Birnessite, Anorthite (sodian), Kaolinite 1A	0.82 ±0.05	2.11±0.04	0.88±0.09	42.5	21.2	36.3	Clay

Table S2. FTIR spectral characteristics of nine selected urban soils.

Wavelength range (cm ⁻¹)	Vibrations	Components	Reference
3600-3750	O–H stretching, “free” hydroxyl	Hydroxyl groups	1
3200-3450	O–H stretching, H-bonded	Carboxyl, alcohols and phenols/amine, and amide groups	2
2800-2950	C–H stretching	Alkanes groups, Aliphatic methyl and methylene groups	3
1800-1950	C=O stretching	Anhydrides	1
1680-1640	C=C stretching	Alkenes group Amides, COO–/aromatics/O–H stretching	4,5
1025-1200	C–H in plane	Aromatics	6

Table S3. Constants and coefficients for determination of pseudo-first-order and pseudo-second-order kinetics models of dimethoate sorption and desorption.

Soil ID	Pseudo-first-order kinetics model				Pseudo-second-order kinetics model			
	$K_{1(Sor)}$	$K_{1(Des)}$	$R^2_{(Sor)}$	$R^2_{(Des)}$	$K_{2(Sor)}$	$K_{2(Des)}$	$R^2_{(Sor)}$	$R^2_{(Des)}$
TAR	1.1E4	7.6E3	0.019	0.031	0.06	0.04	1.00	1.00
FLE	7.6E3	5.7E3	0.090	0.058	0.08	0.03	1.00	1.00
SAL	3.8E3	3.8E3	0.108	0.124	0.02	0.02	0.999	0.999
ATC	7.6E3	4.6E3	0.045	0.125	0.04	0.02	1.00	1.00
FOR	7.6E3	5.7E3	0.035	0.072	0.04	0.03	1.00	1.00
WAB	2.3E4	7.6E3	0.004	0.039	0.08	0.04	1.00	1.00
MAR	1.1E4	7.6E3	0.017	0.033	0.07	0.05	1.00	1.00
WAT	7.6E3	5.7E3	0.036	0.077	0.04	0.03	1.00	1.00
NLT	3.2E4	1.1E4	0.002	0.032	0.14	0.04	1.00	1.00

Sor = Sorption; *Des* = Desorption

References

1. Z. Xing, K. Tian, C. Du, C. Li, J. Zhou and Z. Chen, Agricultural soil characterization by FTIR spectroscopy at micrometer scales: Depth profiling by photoacoustic spectroscopy, *Geoderma*, 2019, **335**, 94–103.
2. M.-H. Bernier, G. J. Levy, P. Fine and M. Borisover, Organic matter composition in soils irrigated with treated wastewater: FTIR spectroscopic analysis of bulk soil samples, *Geoderma*, 2013, **209**, 233–240.
3. J. M. Soriano-Disla, L. J. Janik, R. A. Viscarra Rossel, L. M. Macdonald and M. J. McLaughlin, The performance of visible, near-, and mid-infrared reflectance spectroscopy for prediction of soil physical, chemical, and biological properties, *Appl. Spectros. Rev.*, 2014, **49**, 139–186.
4. F. Calderón, M. Haddix, R. Conant, K. Magrini-Bair and E. Paul, Diffuse-reflectance Fourier-transform mid-infrared spectroscopy as a method of characterizing changes in soil organic matter, *Soil Sci. Soci. Am. J.*, 2013, **77**, 1591–1600.
5. D. Changwen, R. Linker and A. Shaviv, Characterization of soils using photoacoustic mid-infrared spectroscopy, *Appl. Spectros.*, 2007, **61**, 1063–1067.
6. L. J. Janik, J. Skjemstad, K. Shepherd and L. Spouncer, The prediction of soil carbon fractions using mid-infrared-partial least square analysis, *Soil Res.*, 2007, **45**, 73–81.