

**Table S64** Observed and simulated cumulative ammonia (NH<sub>3</sub>) volatilizations from upland soils during the measurement periods, model biases, and management practices of individual fertilizer application cases.

Case code <sup>a</sup>	Site <sup>b</sup>	Period	<i>O</i> <sup>c</sup>	<i>S</i> <sup>c</sup>	RMB <sup>c</sup>	Crop	Irrigation <sup>d</sup> / precipitation	Fertilizer application		
								Type <sup>e</sup>	Method <sup>f</sup>	Dose <sup>g</sup>
U1 <sup>@</sup>	DBW	Oct. 22 to Nov. 4, 2002	15.2	7.50	−50.6	Winter wheat	0/0	ABC	BFT20 <sup>\$</sup>	150
U2 <sup>@</sup>	DBW	Jul. 16 to Jul. 30, 2003	24.1	18.47	−23.4	Summer maize	1.5/0	ABC	B	100
U3	QZ	Oct. 8 to Oct. 19, 1999	18.9	27.72	46.7	Winter wheat	0/0	ABC	BFT20	191.3
U4	QZ	Oct. 18 to Oct. 31, 2000	25.2	22.47	−10.8	Winter wheat	0/3.99	ABC	BFT20	210
U5 <sup>@</sup>	YT	Nov. 8 to Nov. 17, 2013	9.7	10.20	5.2	Winter wheat	0/0.54	ABC	BFT20 <sup>\$</sup>	130
U6	LC	Oct. 11 to Oct. 19, 1999	1.2	4.89	307.8	Winter wheat	0/0	AP, Urea	BFT20 <sup>\$</sup>	130
U7	GC	Mar. 28 to May 6, 2012	11.1	0.83	−92.6	Winter wheat	5 <sup>*</sup> /5.42	AS	B	122
U8	GC	Mar. 28 to May 6, 2012	5.8	0.81	−86.1	Winter wheat	5 <sup>*</sup> /5.42	CF	B	117
U9 <sup>@</sup>	DBW	Apr. 20 to May 4, 2003	29.9	29.59	−1.0	Winter wheat	9/0	Urea	B	150
U10 <sup>@</sup>	DBW	Aug. 4 to Aug. 18, 2003	66.3	44.82	−32.4	Summer maize	1.5/0	Urea	B	200
U11 <sup>@</sup>	DBW	Jul. 18 to Aug. 1, 2004	22.1	29.12	31.8	Summer maize	2/0	Urea	B	100
U12 <sup>@</sup>	DBW	Aug. 4 to Aug. 18, 2004	47.4	44.40	−6.3	Summer maize	2/0	Urea	B	200
U13 <sup>@</sup>	FQU	Jun. 28 to Jul. 10, 1990	25.3	23.62	−6.6	Summer maize	0/2.30	Urea	B	80
U14 <sup>@</sup>	FQU	Jun. 28 to Jul. 10, 1990	9.2	16.22	76.3	Summer maize	0/2.30	Urea	D5–10	80
U15 <sup>@</sup>	FQU	Jun. 29 to Jul. 7, 1998	32.7	36.28	11.0	Summer maize	0/0.21	Urea	B	75
U16 <sup>@</sup>	FQU	Jun. 29 to Jul. 7, 1998	13.4	38.75	189.2	Summer maize	4–6/0.21	Urea	B	75
U17 <sup>@</sup>	FQU	Jul. 19 to Jul. 30, 1998	96.7	102.13	5.6	Summer maize	0/12.00	Urea	B	200

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U18 <sup>@</sup>	FQU	Jul. 19 to Jul. 30, 1998	22.1	41.56	88.1	Summer maize	0/12.00	Urea	D5	200
U19 <sup>@</sup>	FQU	Oct. 11 to Oct. 23, 1998	24.0	12.95	−46.0	Winter wheat	4−6/0.33	Urea	B	120
U20 <sup>@</sup>	FQU	Oct. 11 to Oct. 23, 1998	2.8	7.78	177.7	Winter wheat	4−6/0.33	Urea	BFT5	120
U21 <sup>@</sup>	FQU	Mar. 9 to Mar. 24, 1999	14.6	7.00	−52.1	Winter wheat	0/1.83	Urea	B	100
U22 <sup>@</sup>	FQU	Mar. 9 to Mar. 24, 1999	0.6	2.31	284.7	Winter wheat	4−6/1.83	Urea	B	100
U23 <sup>@</sup>	FQU	Jul. 12 to Jul. 24, 1999	37.8	62.45	65.2	Summer maize	0/0.46	Urea	B	150
U24 <sup>@</sup>	FQU	Jul. 12 to Jul. 24, 1999	18.3	30.84	68.5	Summer maize	0/0.46	Urea	D5	150
U25 <sup>@</sup>	FQU	May 1 to May 15, 2009	27.5	57.16	107.9	Winter wheat	0.8/4.17	Urea	B	113.2
U26 <sup>@</sup>	FQU	Jul. 25 to Aug. 10, 2009	7.6	30.45	300.7	Summer maize	0.8/3.69	Urea	B	140
U27 <sup>@</sup>	FQU	Mar. 26 to Apr. 9, 2010	18.5	10.58	−42.8	Winter wheat	5/0	Urea	B	139.2
U28 <sup>@</sup>	FQU	Jul. 26 to Aug. 5, 2010	44.0	45.29	2.9	Summer maize	0/8.26	Urea	B	174
U29 <sup>@</sup>	FQU	Oct. 2 to Oct. 11, 2010	127.7	115.23	−9.8	Crop interval	0/0	Urea	B	348
U30 <sup>@</sup>	FQU	Mar. 25 to Apr. 8, 2011	10.6	6.62	−37.6	Winter wheat	5/0.94	Urea	Band5	139.2
U31 <sup>@</sup>	FQU	Jun. 18 to Jun. 27, 2012	38.9	30.57	−21.4	Summer maize	6.4/0	Urea	B	174
U32	GC	Mar. 28 to May 6, 2012	15.8	7.14	−54.8	Winter wheat	5 <sup>*</sup> /5.42	Urea	B	140
U33	LC	Jul. 14 to Jul. 24, 1999	41.8	29.28	−29.9	Summer maize	0/0.08	Urea	B	157
U34	LC	Mar. 28 to Apr. 16, 2000	17.1	7.21	−57.8	Winter wheat	5 <sup>*</sup> /0.09	Urea	B	110
U35 <sup>@</sup>	QZ	Jul. 27 to Aug. 8, 1999	42.9	13.66	−68.2	Summer maize	10/0.70	Urea	B	186.3
U36 <sup>@</sup>	QZ	Apr. 4 to Apr. 20, 2000	35.1	19.87	−43.4	Winter wheat	10/1.27	Urea	B	150
U37 <sup>@</sup>	QZ	Jul. 18 to Jul. 31, 2000	63.5	51.72	−18.5	Summer maize	0/4.33	Urea	B	148.3
U38	YT	Jun. 26 to Jul. 14, 2013	59.7	84.68	41.8	Summer maize	0/27.69	Urea	B	175
U39	YT	Aug. 23 to Sep. 3, 2013	16.7	30.45	82.3	Summer maize	3/6.7	Urea	B	150
U40	YT	Mar. 16 to Mar. 29, 2014	7.9	4.01	−49.2	Winter wheat	3/3.72	Urea	B	100
U41	YT	Jun. 21 to Jul. 10, 2014	19.3	28.54	47.9	Summer maize	0/0	Urea	Band5	90

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U42	YT	Jul. 29 to Aug. 13, 2014	28.0	15.29	−45.4	Summer maize	3/0	Urea	B	60
U43	YT	Nov. 5 to Nov. 20, 2014	11.4	3.57	−68.7	Winter wheat	0/0	Urea	BFT20 <sup>s</sup>	130
U44	YJ	Jul. 9 to Jul.19, 2008	3.6	9.87	174.1	Summer maize	0/1.91	Urea	D5–10	60

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<sup>a</sup> U1 to U44 encode the experimental cases following individual application events of synthetic nitrogen fertilizers; the superscript “@” marks the cases with the observations being referred to the model modification/calibration.

<sup>b</sup> The sites are Dongbeiwang (DBW), Fengqiu with uplands (FQU), Guangchuan (GC), Luancheng (LC), Quzhou (QZ), Yanting (YT), and Yongji (YJ).

<sup>c</sup>  $O$  and  $S$  are the cumulative  $\text{NH}_3$  volatilization ( $\text{kg N ha}^{-1}$ ) observed and simulated by the modified CNMM-DNDC, respectively; RMB is the relative model bias (%) of the modified model, which was determined as the relative difference between the simulated and observed values.

<sup>d</sup> The amount of irrigation (cm). For the cases with “\*”, the exact amount of irrigation was not reported and thus was arbitrarily set as the traditional irrigation amount of the FQ site, which was located in the same region. Precipitation denotes total rainfall (cm) during the experimental period(s).

<sup>e</sup> The fertilizers in addition to urea are ammonium bicarbonate (ABC), complex fertilizer (CF), ammonium sulfate (AS), and ammonium monohydric phosphate (AP).

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<sup>f</sup> The application methods are surface broadcast (B), deep point placement (D), band application (Band), and broadcast followed by tillage (BFT).

The figures following D, Band, BFT, and Band are the depth in soil (cm). For the cases with “\$” symbol, exact depth of tillage was not reported, and thus was arbitrarily set as the traditional tillage depth (i.e., 20 cm).

<sup>g</sup> Unit: kg N ha<sup>-1</sup>.