# **Table S6** Observed and simulated cumulative ammonia (NH3) volatilizations from upland soils during measurement periods, model biases, and management practices of individual fertilizer application cases.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Case code a | Site b | Period | *O* c | *S* c | RMB c | Crop | Irrigation d/  precipitation | Fertilizer application | | |
| Type e | Method f | Dose g |
| U1 @ | DBW | Oct. 22 to Nov. 4, 2002 | 15.2 | 7.50 | –50.6 | Winter wheat | 0/0 | ABC | BFT20$ | 150 |
| U2 @ | 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 @ | YT | Nov. 8 to Nov. 17, 2013 | 9.7 | 10.20 | 5.2 | Winter wheat | 0/0.54 | ABC | BFT20$ | 130 |
| U6 | LC | Oct. 11 to Oct. 19, 1999 | 1.2 | 4.89 | 307.8 | Winter wheat | 0/0 | AP, Urea | BFT20$ | 130 |
| U7 | GC | Mar. 28 to May 6, 2012 | 11.1 | 0.83 | –92.6 | Winter wheat | 5 \*/5.42 | AS | B | 122 |
| U8 | GC | Mar. 28 to May 6, 2012 | 5.8 | 0.81 | –86.1 | Winter wheat | 5 \*/5.42 | CF | B | 117 |
| U9 @ | DBW | Apr. 20 to May 4, 2003 | 29.9 | 29.59 | –1.0 | Winter wheat | 9/0 | Urea | B | 150 |
| U10 @ | DBW | Aug. 4 to Aug. 18, 2003 | 66.3 | 44.82 | –32.4 | Summer maize | 1.5/0 | Urea | B | 200 |
| U11 @ | DBW | Jul. 18 to Aug. 1, 2004 | 22.1 | 29.12 | 31.8 | Summer maize | 2/0 | Urea | B | 100 |
| U12 @ | DBW | Aug. 4 to Aug. 18, 2004 | 47.4 | 44.40 | –6.3 | Summer maize | 2/0 | Urea | B | 200 |
| U13 @ | FQU | Jun. 28 to Jul. 10, 1990 | 25.3 | 23.62 | –6.6 | Summer maize | 0/2.30 | Urea | B | 80 |
| U14 @ | FQU | Jun. 28 to Jul. 10, 1990 | 9.2 | 16.22 | 76.3 | Summer maize | 0/2.30 | Urea | D5–10 | 80 |
| U15 @ | FQU | Jun. 29 to Jul. 7, 1998 | 32.7 | 36.28 | 11.0 | Summer maize | 0/0.21 | Urea | B | 75 |
| U16 @ | FQU | Jun. 29 to Jul. 7, 1998 | 13.4 | 38.75 | 189.2 | Summer maize | 4–6/0.21 | Urea | B | 75 |
| U17 @ | FQU | Jul. 19 to Jul. 30, 1998 | 96.7 | 102.13 | 5.6 | Summer maize | 0/12.00 | Urea | B | 200 |
| U18 @ | FQU | Jul. 19 to Jul. 30, 1998 | 22.1 | 41.56 | 88.1 | Summer maize | 0/12.00 | Urea | D5 | 200 |
| U19 @ | FQU | Oct. 11 to Oct. 23, 1998 | 24.0 | 12.95 | –46.0 | Winter wheat | 4–6/0.33 | Urea | B | 120 |
| U20 @ | FQU | Oct. 11 to Oct. 23, 1998 | 2.8 | 7.78 | 177.7 | Winter wheat | 4–6/0.33 | Urea | BFT5 | 120 |
| U21 @ | FQU | Mar. 9 to Mar. 24, 1999 | 14.6 | 7.00 | –52.1 | Winter wheat | 0/1.83 | Urea | B | 100 |
| U22 @ | FQU | Mar. 9 to Mar. 24, 1999 | 0.6 | 2.31 | 284.7 | Winter wheat | 4–6/1.83 | Urea | B | 100 |
| U23 @ | FQU | Jul. 12 to Jul. 24, 1999 | 37.8 | 62.45 | 65.2 | Summer maize | 0/0.46 | Urea | B | 150 |
| U24 @ | FQU | Jul. 12 to Jul. 24, 1999 | 18.3 | 30.84 | 68.5 | Summer maize | 0/0.46 | Urea | D5 | 150 |
| U25 @ | FQU | May 1 to May 15, 2009 | 27.5 | 57.16 | 107.9 | Winter wheat | 0.8/4.17 | Urea | B | 113.2 |
| U26 @ | FQU | Jul. 25 to Aug. 10, 2009 | 7.6 | 30.45 | 300.7 | Summer maize | 0.8/3.69 | Urea | B | 140 |
| U27 @ | FQU | Mar. 26 to Apr. 9, 2010 | 18.5 | 10.58 | –42.8 | Winter wheat | 5/0 | Urea | B | 139.2 |
| U28 @ | FQU | Jul. 26 to Aug. 5, 2010 | 44.0 | 45.29 | 2.9 | Summer maize | 0/8.26 | Urea | B | 174 |
| U29 @ | FQU | Oct. 2 to Oct. 11, 2010 | 127.7 | 115.23 | –9.8 | Crop interval | 0/0 | Urea | B | 348 |
| U30 @ | FQU | Mar. 25 to Apr. 8, 2011 | 10.6 | 6.62 | –37.6 | Winter wheat | 5/0.94 | Urea | Band5 | 139.2 |
| U31 @ | 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 \*/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 \*/0.09 | Urea | B | 110 |
| U35 @ | QZ | Jul. 27 to Aug. 8, 1999 | 42.9 | 13.66 | –68.2 | Summer maize | 10/0.70 | Urea | B | 186.3 |
| U36 @ | QZ | Apr. 4 to Apr. 20, 2000 | 35.1 | 19.87 | –43.4 | Winter wheat | 10/1.27 | Urea | B | 150 |
| U37 @ | 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 |
| 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$ | 130 |
| U44 | YJ | Jul. 9 to Jul.19, 2008 | 3.6 | 9.87 | 174.1 | Summer maize | 0/1.91 | Urea | D5–10 | 60 |

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

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

c *O* and *S* are the cumulative NH3 volatilization (kg N ha–1) which are observed and simulated by the modified CNMM-DNDC model, respectively; RMB is the relative model biases (%) of the modified model, each of which was determined as the relative difference between the simulated and observed values.

d The amount of irrigation (cm). For the cases with “\*” symbol, 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).

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

f 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).

g Unit: kg N ha–1.