

**Table S1** Equations of the direct processes calculating NH<sub>3</sub> volatilization from upland soils in the original and modified CNMM-DNDC model.

| Equations   | Description  |        |
|---|--|--------|
| <b><i>Original CNMM-DNDC model</i></b>  |  |        |
| <b>Urea hydrolysis</b>  |  |        |
| $d[\text{NH}_4^+]_j/dt = -d[\text{urea}]_j/dt$  | Urea hydrolysis rate   | Eq. 1  |
| $= f_T f_{\text{SOC}} [\text{urea}]_j$  |  |        |
| $f_T = 0.0364e^{0.0805T_{\text{soil}}}$   | Effect of soil temperature on urea hydrolysis                | Eq. 2  |
| $f_{\text{SOC}} = 0.01[\text{SOC}]_j^{-1}$  | Effect of soil temperature on urea hydrolysis                | Eq. 3  |
| <b>ABC decomposition</b>  |  |        |
| $f_{\text{ABC\_dec}} = f_{\text{pH}} f_{\text{dp}}$   | ABC decomposition rate                                       | Eq. 4  |
| $f_{\text{pH}} = 0.1\text{pH} - 0.5$  | Effect of soil pH on ABC decomposition                       | Eq. 5  |
| $f_{\text{dp}} = 6.0 \times 10^{-3.6735j/q-0.7551}$   | Effect of soil depth on ABC decomposition                    | Eq. 6  |
| $\text{NH}_3\text{_{flux}(j)} = f_{\text{ABC\_dec}} [\text{NH}_4\text{HCO}_3]_j$  | NH <sub>3</sub> volatilization from ABC decomposition        | Eq. 7  |
| <b>NH<sub>3</sub> volatilization</b>  |  |        |
| $\text{Flux}(\text{NH}_3)_{\text{upland}(j)} = 0.25 f_{\text{wind}} f_{\text{depth}} f_{\text{temp}} [\text{NH}_3(\text{l})]_j$ | NH <sub>3</sub> flux from uplands                            | Eq. 8  |
| $f_{\text{wind}} = 1.5S_{\text{wind}}/(1.0 + S_{\text{wind}})$  | Effect of wind speed on NH <sub>3</sub> volatilization       | Eq. 9  |
| $f_{\text{depth}} = (d_s/d_1 - j)/(d_s/d_1)$  | Effect of soil depth on NH <sub>3</sub> volatilization       | Eq. 10 |
| $f_{\text{temp}} = T_{\text{soil}}/(50 + T_{\text{soil}})$  | Effect of soil temperature on NH <sub>3</sub> volatilization | Eq. 11 |
| <b><i>Modified CNMM-DNDC model</i></b>  |  |        |
| <b>Urea hydrolysis</b>  |  |        |
| $d[\text{NH}_4^+]_j/dt = -d[\text{urea}]_j/dt$  | Urea hydrolysis rate   | Eq. 12 |
| $= f_T f_{\text{SOC}} f_{\text{SM}} [\text{urea}]_j$  |  |        |
| $f_T = 0.45e^{0.025T_{\text{soil}}}$  | Effect of soil temperature on urea hydrolysis                | Eq. 13 |

$$f_{SM} = \text{WFPS}/\text{PORE}$$

Effect of soil moisture on urea hydrolysis Eq. 14

$$f_{SOC} = 0.01[\text{SOC}]_j^{-1}$$

Effect of soil temperature on urea hydrolysis Eq. 15

### ABC decomposition

$$f_{ABC\_dec} = f_{pH} f_{dp} f_{T\_s\_ABC}$$

ABC decomposition rate Eq. 16

$$f_{pH} = 0.1\text{pH} - 0.5$$

Effect of soil pH on ABC decomposition Eq. 17

$$f_{dp} = 6.0 \times 10^{-3.6735j/q-0.7551}$$

Effect of soil depth on ABC decomposition Eq. 18

$$f_{T\_s\_ABC} = T_{soil}/(30 + T_{soil})$$

Effect of soil temperature on ABC decomposition Eq. 19

$$\text{NH}_3\_flux(j) = f_{ABC\_dec} [\text{NH}_4\text{HCO}_3]_j$$

NH<sub>3</sub> volatilization from ABC decomposition Eq. 20

### NH<sub>3</sub> volatilization

$$\text{Flux}(\text{NH}_3)_{\text{upland}(j)}$$

NH<sub>3</sub> flux from uplands Eq. 21

$$= 3.6 f_{wind} f_{depth} f_{temp} f_{canopy} f_{clay} f_{water} f_{rain} [\text{NH}_3(l)]_j$$

$$f_{wind} = 0.1 + 1.5 S_{wind}/(1 + S_{wind})$$

Effect of wind speed on NH<sub>3</sub> volatilization Eq. 22

$$f_{depth} = 0.5^{d_{soil}/0.03}$$

Effect of soil depth on NH<sub>3</sub> volatilization Eq. 23

$$f_{temp} = 0.1 + 2.0 T_{soil}/(45 + T_{soil})$$

Effect of soil temperature on NH<sub>3</sub> volatilization Eq. 24

$$f_{canopy} = 0.4e^{-0.15lai} + 0.6$$

Effect of dry canopy on NH<sub>3</sub> volatilization Eq. 25

$$f_{clay} = e^{-0.06cl}$$

Effect of soil clay content on NH<sub>3</sub> volatilization Eq. 26

$$f_{water} = 0.45e^{-10\text{WFPS}_j/\text{PORE}} + 0.55$$

Effect of soil moisture on NH<sub>3</sub> volatilization Eq. 27

$$f_{rain} = 0.65e^{-1.0laiP} + 0.35$$

Effect of rain wetting canopy on NH<sub>3</sub> volatilization Eq. 28