



Fig. S1 CNMM-DNDC model-included processes determining ammonium (NH_4^+), ammonia (NH_3) concentrations in the liquid phase of a soil, and ammonium bicarbonate decomposition (ABC), and thus volatilization of this nitrogenous gas in the uplands. This figure was drawn by decoding the original and revised Catchment Nutrient Management Model - DeNitrification DeComposition (i.e., CNMM-DNDC) model. $\text{NH}_4^+(\text{clay})$ denotes the NH_4^+ adsorbed by clay minerals. $\text{NH}_4^+(\text{l})$ and $\text{NH}_3(\text{l})$ are referred to as dissolved NH_4^+ and NH_3 , respectively, in the liquid phase of a soil. Bold word(s) aside arrow(s) indicate(s) the nitrogen transfer/transformation process(es). Italic word(s) aside arrow(s) is/are the regulating factor(s) for the corresponding process(es). The influencing factors with their parameters/parameterizations/definitions fully inherited from the original DNDC95 (<http://www.dnnc.sr.unh.edu/>) with minor changes by Cui et al. (2014) are shown in black, and those newly added/calibrated in the studies of Dubache et al. (2019) and Li et al. (2019) are displayed in red.

Reference

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- Li, S., Zheng, X., Zhang, W., Han, S., Deng, J., Wang, K., Wang, R., Yao, Z., Liu, C., 2019. Modeling ammonia volatilization following the application of synthetic fertilizers to cultivated uplands with calcareous soils using an improved DNDC biogeochemistry model. *Sci. Total Environ.* 660, 931–946. <http://dx.doi.org/10.1016/j.scitotenv.2018.12.379>
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