Supplement of Geosci. Model Dev., 16, 1641–1659, 2023
https://doi.org/10.5194/gmd-16-1641-2023-supplement

Geoscientific Model Development
Open Access
EGU

Supplement of

A dynamic ammonia emission model and the online coupling with WRF–Chem (WRF–SoilN–Chem v1.0): development and regional evaluation in China

Chuanhua Ren et al.

Correspondence to: Xin Huang (xinhuang@nju.edu.cn)

Table S1. Activity data set and source

Activity Data Set and Its Description	Data Source
Synthetic fertilizer application (synthetic fertilizer consumption)	NBSC: 12-5 Fertilizer application rates for agricultural use
Agriculture soil (cultivated areas)	NBSC: 12-5 Area of irrigated arable land
Nitrogen-fixing crop (cultivated areas)	NBSC: 12-1 Area of crops sown
Compost of crop residues (mass composted)	NBSC: 12-10 Production of major agricultural products and production-to-residue ratios (Lal, 2005)
Livestock wastes (animal population)	China animal husbandry and veterinary yearbook 2020: Year-end livestock stock statistics by region
Biomass burning (burned biomass or burned area)	MODIS burned area product (MCD45A1)
Excrement of rural population (rural population using tatty latrine)	NBSC: 2-14 Population by region
Chemical industry (production)	NBSC: 13-12 Production of industrial products
Waste disposal (waste amount)	NBSC: 8-15 Solid waste disposal and utilization
Traffic sources (vehicle population)	NBSC: 16-2 Basic information on the transport sector

NBSC: National Bureau of Statistics of China (2020)

Table S2. EFs, Expressed as Percentage of Volatilized NH_3-N from Applied Fertilizer-N, and Static Correction Coefficients for Different N Fertilizer Categories.

Fertilizer Categories	Measured EFs		Coerrection Coefficients	
	Acid Soil	Alkaline Soil	CF_{rate} [a]	CF_{method} [b]
Urea	8.8[c]	30.1[c]	1.18	0.32
ABC	18.2[d]	39.1[d]	1.18	0.32
AN	1.6[e]	3.3[e]	1.18	0.32
Others	1.4[e]	2.0[e]	1.18	0.32

[a]Values are derived from *Li et al. (2002), Song et al. (2004), and Fan et al. (2006).*

[b]Values are derived from *Lu et al. (1980), Qu (1980), Fillery et al. (1986), Zhang and Zhu (1992), Li and Ma (1993), and Cai et al. (2002)*

[c]Measurement results of *Zhu et al. (1989).*

[d]Measurement results of *Cai et al. (1986).*

[e]Values recommended by EEA (2019).

Table S3. EFs in the estimation of ammonia emission from livestock waste management

Parameters	EF_{house_slurry}	EF_{house_solid}	$EF_{outside}$	$EF_{storage\_slurry}$	$EF_{storage\_solid}$	EF_{spread_slurry}	EF_{spread_solid}
Free-range system							
Beef<1 year	7	7	53	20	27	55	79
Beef>1 year	14	14	53	20	27	55	79
Dairy cows<1 year	7	7	53	20	27	55	79
Dairy cows>1 year	14	14	30	20	27	55	79
Goat<1 year	7	7	53	20	27	55	79
Goat>1 year	14	14	75	28	28	90	81
Sheep<1 year	7	7	53	20	27	55	79
Sheep>1 year	14	14	75	28	28	90	81
Sow	14.7	14.7	0	14	45	40	81
Weaner	15.6	15.6	0	14	45	40	81
Fattening pig	10.2	10.2	0	14	45	40	81
Horse	14	14	0	35	35	90	81
Donkey	14	14	0	35	35	90	81
Mule	14	14	0	35	35	90	81
Camel	14	14	0	35	35	90	81
Laying hen	45.2	45.2	69	0	14	0	63
Laying duck	45.2	45.2	54	0	24	0	63
Laying goose	45.2	45.2	54	0	24	0	63
Broilers	40.3	40.3	66	0	17	0	63
Meat duck	40.3	40.3	54	0	24	0	63
Meat goose	40.3	40.3	54	0	24	0	63
Intensive system							
Beef<1 year	7	7	53	15.8	4.2	55	79
Beef>1 year	14	14	53	15.8	4.2	55	79
Dairy cows<1 year	7	7	53	15.8	4.2	55	79
Dairy cows>1 year	14	14	30	15.8	4.2	55	79
Goat<1 year	7	7	53	15.8	4.2	55	79
Goat>1 year	14	14	75	15.8	4.2	90	81
Sheep<1 year	7	7	53	15.8	4.2	55	79
Sheep>1 year	14	14	75	15.8	4.2	90	81
Sow	14.7	14.7	0	3.8	4.6	40	81
Weaner	15.6	15.6	0	3.8	4.6	40	81
Fattening pig	10.2	10.2	0	3.8	4.6	40	81
Horse	14	14	0	15.8	4.2	90	81
Donkey	14	14	0	15.8	4.2	90	81
Mule	14	14	0	15.8	4.2	90	81

Camel	14	14	0	15.8	4.2	90	81
Laying hen	0	35.9	69	0	3.7	0	63
Laying duck	0	35.9	54	0	3.7	0	63
Laying goose	0	35.9	54	0	3.7	0	63
Broilers	0	40.3	66	0	0.8	0	63
Meat duck	0	40.3	54	0	0.8	0	63
Meat goose	0	40.3	54	0	0.8	0	63
Grazing system							
Beef<1 year	7	7	6	20	27	55	79
Beef>1 year	14	14	6	20	27	55	79
Dairy cows<1 year	7	7	6	20	27	55	79
Dairy cows>1 year	14	14	10	20	27	55	79
Goat<1 year	7	7	6	20	27	55	79
Goat>1 year	14	14	9	28	28	90	90
Sheep<1 year	7	7	6	20	27	55	79
Sheep>1 year	14	14	9	28	28	90	90
Horse	14	14	35	35	35	90	90
Donkey	14	14	35	35	35	90	90
Mule	14	14	35	35	35	90	90
Camel	14	14	35	35	35	90	90

Table S1. Overview of Available Models for Fertilizer Emissions.

Reference	Fertilizer	Parameters	Model Type
Fenn and Kissel (1975)	Urea, nitrogen solutions	Time, temperature, application rate	Regression
Alkanani and Mackenzie (1992)	Urea, UAN	Temperature, thermodynamic force, wind velocity, soil surface roughness, adsorption and desorption rate constants	Mechanistic
Ismail et al. (1991)	Urea solution	Soil temperature, application rate, initial soil moisture content, soil pH, application depth	Regression
Kirk and Nye (1991)	Urea	Time, soil moisture content, diffusion factor in soil, vertical distance	Mechanistic
Roelle and Aneja (2002)	Hog slurry	Soil temperature	Regression
Sogaard et al. (2002)	Cattle and pig Slurry	Soil water content, air temp, wind speed, slurry type, dry matter content of slurry, TAN content of slurry, application method, application rate	Mechanistic
Huijsmans et al. (2003)	Slurry	Air temperature, application rate, application method, content of N in slurry, wind speed	Mechanistic
Vira et al. (2019)	Fertilizer and livestock waste	Temperature, precipitation, soil moisture, wind speed, spreading of TAN, application rate	Mechanistic

Soil temperature CF deriving:

Based on the Gibbs free energy equation and the form of correction factor proposed by Gyldenkaerne et al. (2005), the effect of soil temperature on ammonia emission should be exponential (Roelle and Aneja, 2005). And since ammonia emission is influenced by surface temperature and soil temperature gradient, we consider the correction factor equation for soil as equation (1) and (2). Then we combined the activity level data above and multiple factors of temperature, wind speed and precipitation and soil moisture to obtain an equation with coefficients that were fitted to the flux data in April to obtain the coefficients in equation (3). The results of fitting meteorological parameters to ammonia emission fluxes is shown in Figure S1.

$$CF_{soil_T} = CF_{soilT-gradient} \times CF_{soilT-surface} \quad (1)$$

$$CF_{soil_T} = e^{(a1 \times \Delta soil_T + b1)} \times e^{(a2 \times soilT + b2)} \quad (2)$$

$$CF_{soil_T} = e^{(0.093 \times \Delta soil_T - 0.97 + 0.018 \times soil_T)} \quad (3)$$

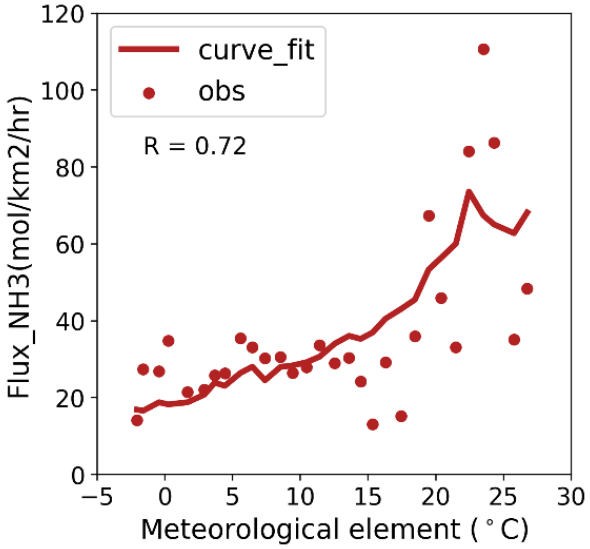

Figure S1. Results of fitting meteorological parameters to ammonia emission fluxes.

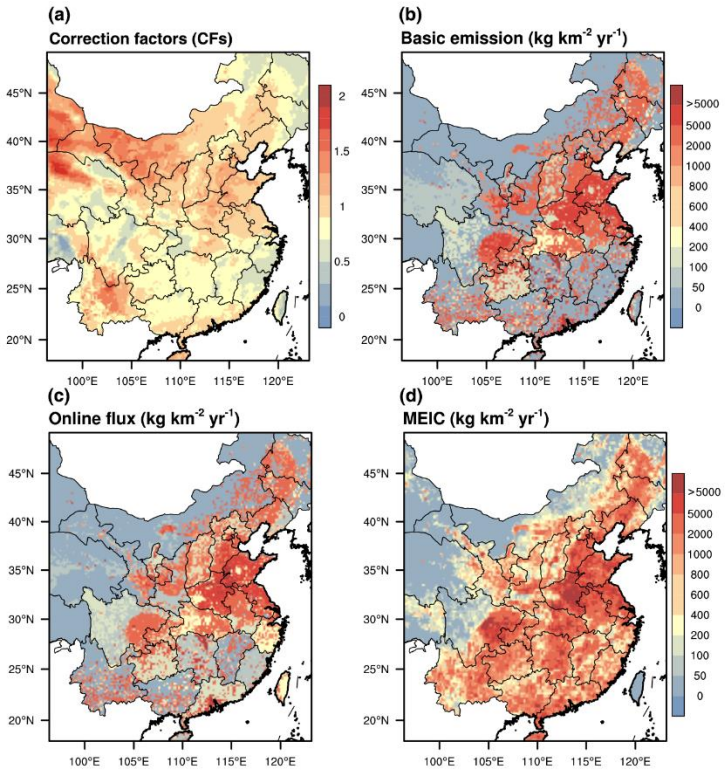

Figure S2. (a) The annual mean CFs, (b) the spatial distribution of basic NH_3 emission, (c) online NH_3 emission, and (d) traditional MEIC NH_3 emission inventory in 2019 for east China.

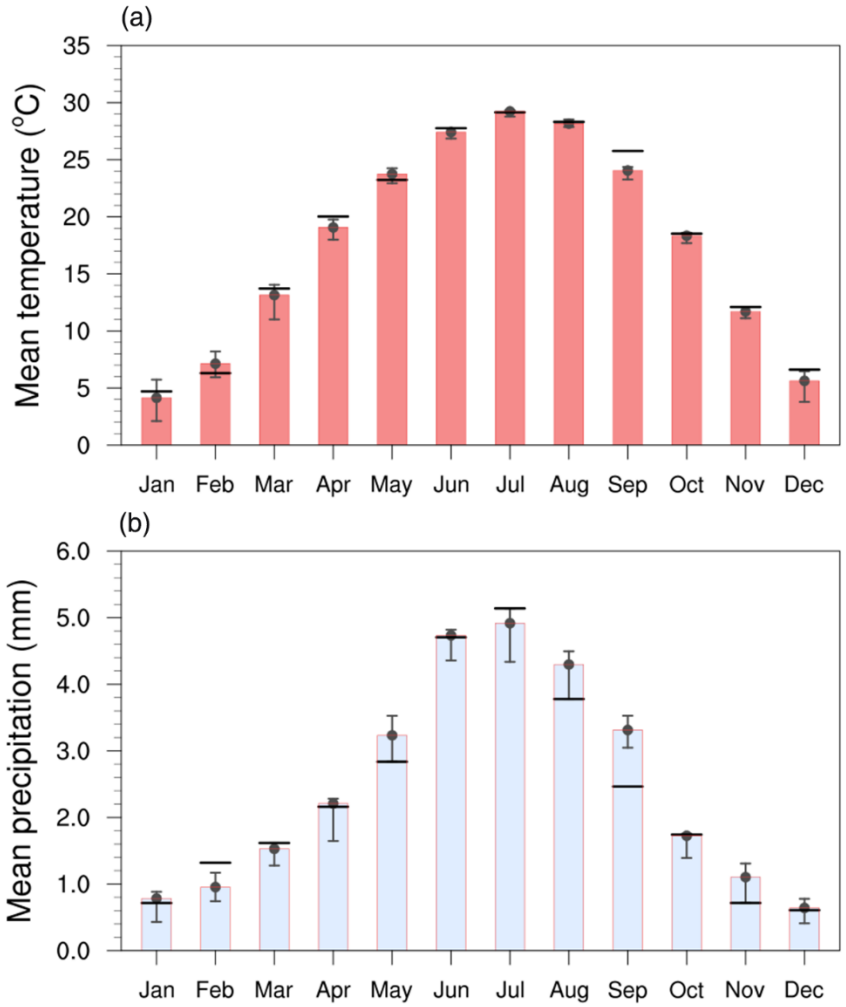

Figure S3. (a) Seasonal pattern of monthly averaged near surface temperature in eastern China (18°N–50°N, 95°E–131°E) during 2010-2019. The lower and upper points of vertical lines show the 25th and 75th percentiles, respectively. The black horizontal line represents mean value in 2019. (b) is same as (a) but for mean precipitation.

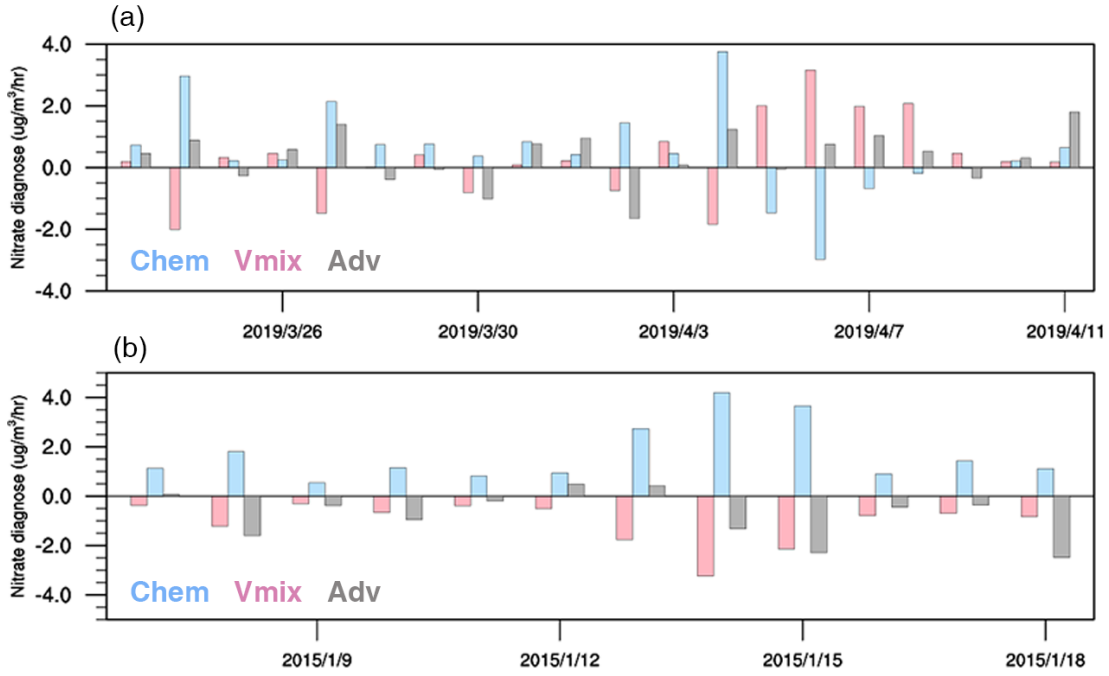

Figure S4. Daily variation of nitrate changes due to chemical production (chem) and PBL evolution (vmix) and advection (adv) calculated from WRF-Chem analysis for the (a) Nanjing and (b) Beijing cases, respectively.

Reference

Alkanani, T. and Mackenzie, A. F.: Effect of Tillage Practices and Hay Straw on Ammonia Volatilization from Nitrogen-Fertilizer Solutions, Can J Soil Sci, 72, 145-157, https://doi.org/10.4141/cjss92-014, 1992.

Cai, G. X., Chen, D. L., Ding, H., Pacholski, A., Fan, X. H., and Zhu, Z. L., Nitrogen losses from fertilizers applied to maize, wheat and rice in the North China Plain, Nutr. Cycl. Agroecosyst., 63, 187–195, https://doi.org/10.1023/A:1021198724250, 2002.

European Environment Agency (EEA), EMEP/EEA air pollutant emission inventory guidebook 2019, Tech. Rep. 13/2019, Copenhagen, 2019.

Fan, X. H., Song, Y. S., Lin, D. X., Yang, L. Z., and Zhou, J. M., Ammonia volatilization losses from urea applied to wheat on a paddy soil in Taihu Region, China [in Chinese], Pedosphere, 15(1), 59–65, 2005.

Fenn, L. B. and Kissel, D. E.: Ammonia Volatilization from Surface Applications of Ammonium-Compounds on Calcareous Soils .4. Effect of Calcium-Carbonate Content, Soil Sci Soc Am J, 39, 631-633, https://doi.org/10.2136/sssaj1975.03615995003900040019x, 1975.

Fillery, I. R. P., Simpson, J. R., and Dedatta, S. K.: Contribution of Ammonia Volatilization to Total Nitrogen Loss after Applications of Urea to Wetland Rice Fields, Fert Res, 8, 193-202, https://doi.org/10.1007/Bf01048620, 1986.

Gyldenkaerne, S., Skjoth, C. A., Hertel, O., and Ellermann, T.: A dynamical ammonia emission parameterization for use in air pollution models, J Geophys Res-Atmos, 110, https://doi.org/10.1029/2004jd005459, 2005.

Huijsmans, J. F. M., Hol, J. M. G., and Vermeulen, G. D.: Effect of application method, manure characteristics, weather and field conditions on ammonia volatilization from manure applied to arable land, Atmos Environ, 37, 3669-3680, https://doi.org/10.1016/S1352-2310(03)00450-3, 2003.

Ismail, K. M., Wheaton, F. W., Douglass, L. W., and Potts, W.: Modeling Ammonia Volatilization from Loamy Sand Soil Treated with Liquid Urea (Correction of Transactions of the Asae, Vol 34, No 3, Pg 756, 1991), T Asae, 34, 756-763, 1991.

Kirk, G. J. D. and Nye, P. H.: A Model of Ammonia Volatilization from Applied Urea .5. The Effects of Steady-State Drainage and Evaporation, J Soil Sci, 42, 103-113, https://doi.org/10.1111/j.1365-2389.1991.tb00095.x, 1991.

Lal, R.: World crop residues production and implications of its use as a biofuel, Environ Int, 31, 575-584, https://doi.org/10.1016/j.envint.2004.09.005, 2005.

Li, G., Li, B., and Chen, D.: Ammonia volatilization from large field planted with winter wheat and summer maize [in Chinese], Acta Agric. Boreali Sin., 17(1), 76–81, 2002.

Li, S., and Ma, S., Ammonia volatilization from calcareous soil II. The relationship between ammonia loss from N fertilizers and applied methods [in Chinese], Agric. Res. Arid Areas, 11, 130–134, 1993.

Lu, D., Liu, X., and Wu, C., The research on conditions affecting the volatilization of ammonium bicarbonate on the calcareous soil and prevention measures [in Chinese], Shaanxi J. Agric. Sci., 6, 7–10, 1980.

Qu, X., The research on the loss from ammonium nitrogen fertilizer on the calcareous soil (in Chinese), Soils Fert., 3, 31–35, 1980.

Roelle, P. A. and Aneja, V. P.: Characterization of ammonia emissions from soils in the upper coastal plain, North Carolina, Atmos Environ, 36, 1087-1097, https://doi.org/10.1016/S1352-2310(01)00355-7, 2002.

Roelle, P. A. and Aneja, V. P.: Modeling of ammonia emissions from soils, Environ Eng Sci, 22, 58-72, https://doi.org/10.1089/ees.2005.22.58, 2005.

Sogaard, H. T., Sommer, S. G., Hutchings, N. J., Huijsmans, J. F. M., Bussink, D. W., and Nicholson, F.: Ammonia volatilization from field-applied animal slurry - the ALFAM model, Atmos Environ, 36, 3309-3319, https://doi.org/10.1016/S1352-2310(02)00300-X, 2002.

Song, Y., Fan, X., and Lin, D., Ammonia volatilation from paddy fields in the Taihu lake region and its influencing factors [in Chinese], Acta Pedol. Sin., 41(2), 265–269, 2004.

Vira, J., Hess, P., Melkonian, J., and Wieder, W. R.: An improved mechanistic model for ammonia volatilization in Earth system models: Flow of Agricultural Nitrogen version 2 (FANv2), Geosci Model Dev, 13, 4459-4490, https://doi.org/10.5194/gmd-13-4459-2020, 2019.

Zhang, S., and Zhu, Z., Losses of urea-Nitrogen applied to maize grown on a calcareous fluvo-aquic soil in North China Plain, Pedosphere, 2(2), 171–178, 1992.