Estimating the agricultural fertilizer NH_3 emission in China based on the bi-directional flux parameterization for air quality models

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Outline

- Background
- Objective
- Method
- Pre-work
- Results
- On-going work

Background

- 1. Smog or haze has become the hottest topic to the publics and received a great concern from our governments, especially in $PM_{2.5}$.

- 2. Secondary non-organic aerosol (SNA) is major component of $PM_{2.5}$ in haze days(He et al., 2012),NH_3 plays an important role in SNA formation process. China is one of the largest countries for NH_3 emission, about 23% (2005, EDGARv4.1). The major contributors are fertilizer use and livestock.

Background

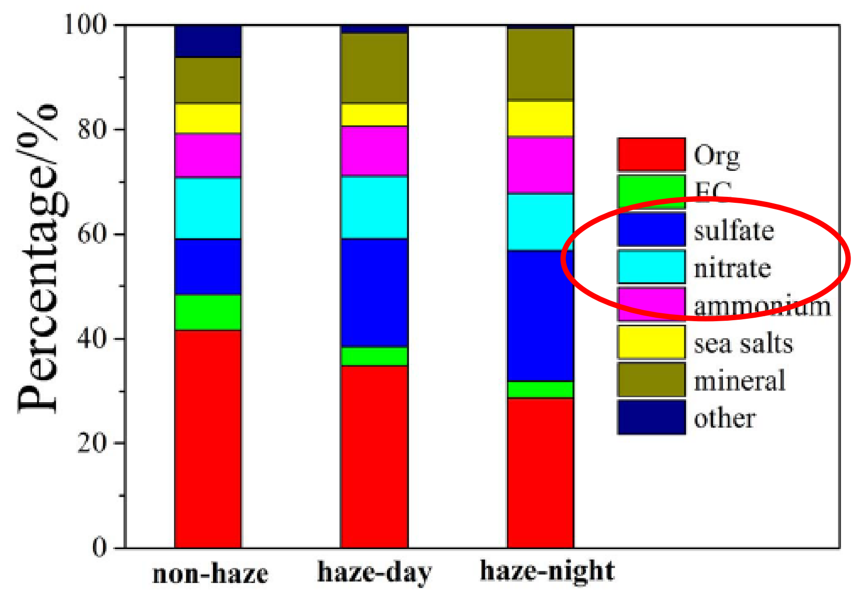
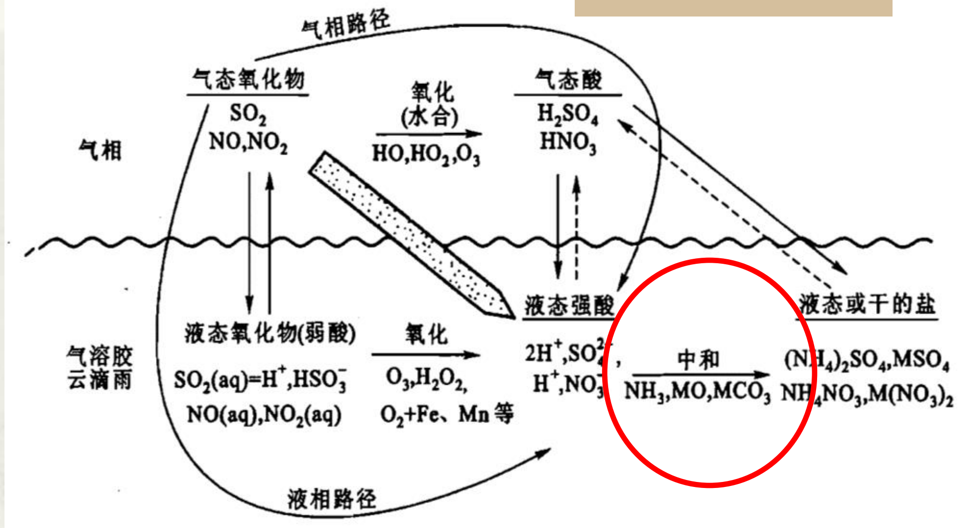
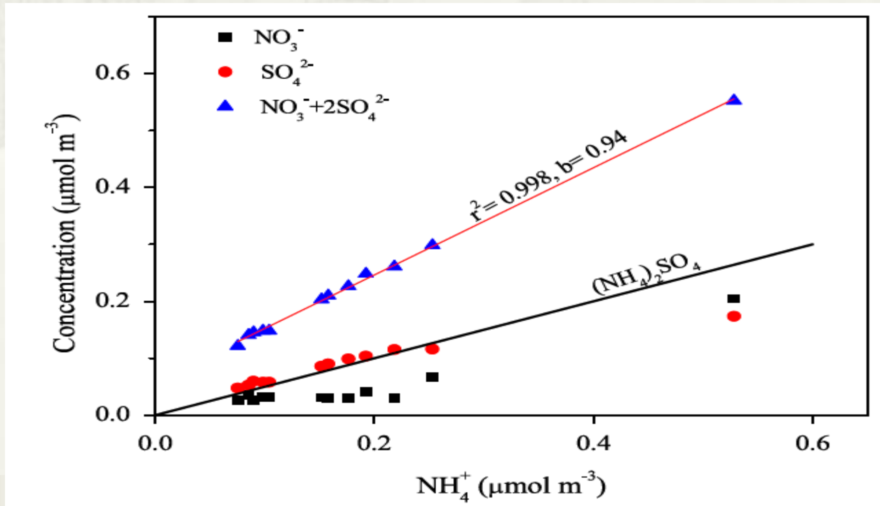


Figure 6 | Mass fraction of different chemical compositions in $PM_{2.5}$ in Beijing station. Non-haze, haze-day, and haze-night represent the sampling times of 12:00 on Jan. 9th, 12:00 on Jan. 12th, and 00:00 on Jan. 13th, 2013, respectively.

(source: He et al., Scientific Reports, 2010)

SNA formation

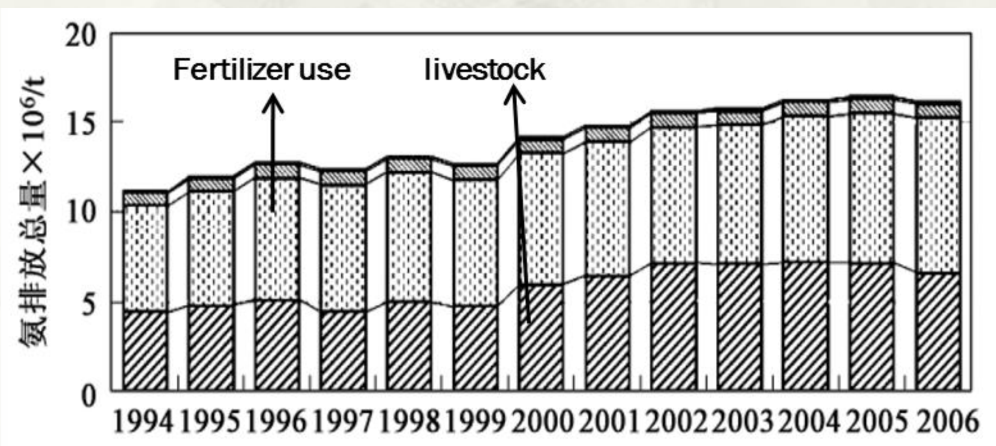




- Secondary non-organic aerosol (SNA) is major component of $PM_{2.5}$ in haze days
- NH_3 plays an important role in SNA formation process

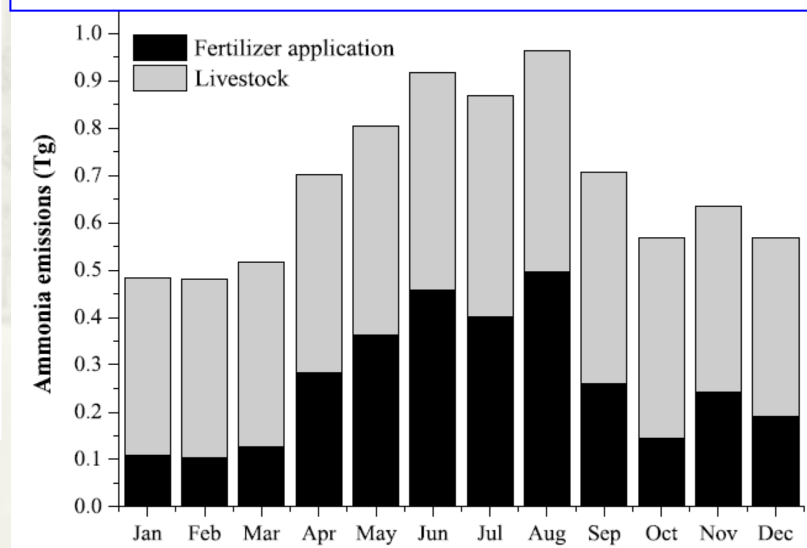
Background

- 3. Limited attention has been given to the agricultural emissions and their impact on air quality. The current emission inventory of NH_3 for China is mainly based on fixed emission factors. Large uncertainty still exists for time and spatial distribution.



Dong et al., Environment Science, 2010

$$EF_i = EF_{0i} \times CF_{pH} \times CF_{rate} \times CF_T \times CF_{method}$$



Huang et al., GB, 2012

Challenge and objective

- Anthropogenic source is easy to control compared with the agricultural emission; High uncertainties associated with agricultural emission inventories have been identified as one of the major challenges in air quality studies.
- Our goal is to find a way to develop an updated and detailed agricultural emission inventory in China(Mainly in fertilizer use)

Application of bidirectional CMAQ in US

Like most dry deposition models, the bidirectional flux model is based on an electrical resistance analog. The total flux between the plant canopy and the overlying atmosphere is the sum of two bidirectional pathways, to the leaf stomata (Fst) and the soil (Fg), and one uni-directional deposition pathway, to the leaf cuticle (Fcut).

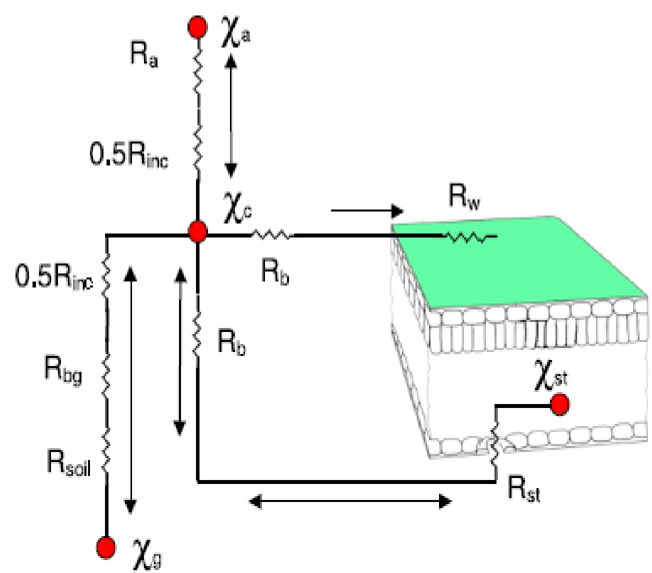
$$F_t = \frac{(\chi_c - \chi_a)}{R_a + 0.5^* R_{inc}} = F_g + F_{st} + F_{cut},$$

and the component fluxes are

$$F_g = \frac{(\chi_g - \chi_c)}{0.5^* R_{inc} + R_{bg} + R_{soil}}$$

$$F_{st} = \frac{(\chi_s - \chi_c)}{R_b + R_{st}}$$

$$F_{cut} = \frac{\chi_c}{R_b + R_w}$$

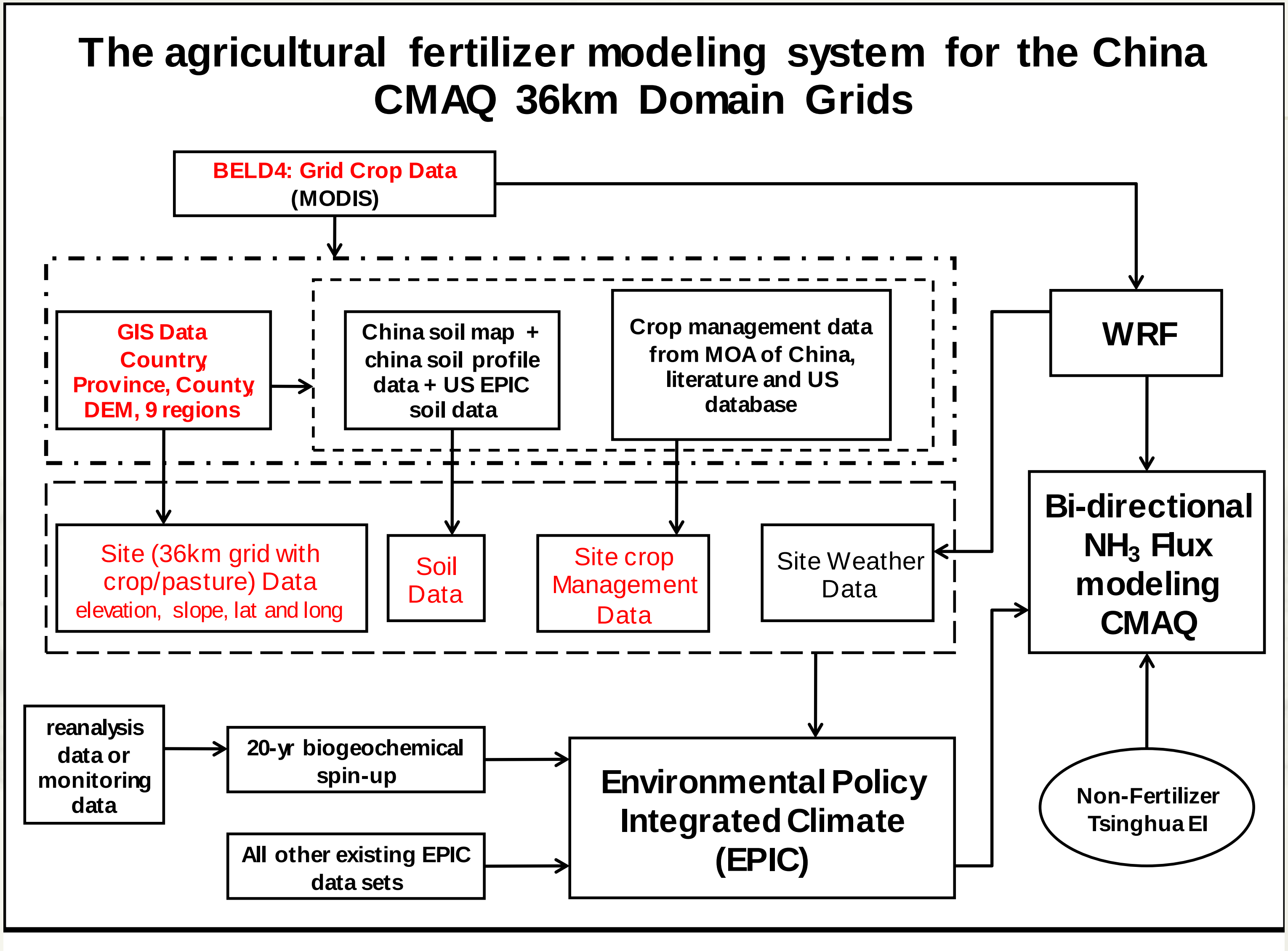


-ww-	Resistance to deposition
R_a	Aerodynamic resistance
R_b	Laminar boundary layer resistance
R_{inc}	In-canopy aerodynamic resistance
R_{bg}	Ground laminar boundary layer resistance
R_w	Cuticular resistance
R_{st}	Stomatal resistance
χ_a	Atmospheric concentration
χ_c	Canopy compensation point
χ_g	Soil compensation point concentration
χ_{st}	Stomatal compensation point concentration
R_{soil}	Soil resistance

Figure 1. Resistance model schematic for bidirectional NH_3 flux with leaf and soil compensation point concentrations.

Source :Jonathan E. Pleim,2013

Method: Structure of the system for China



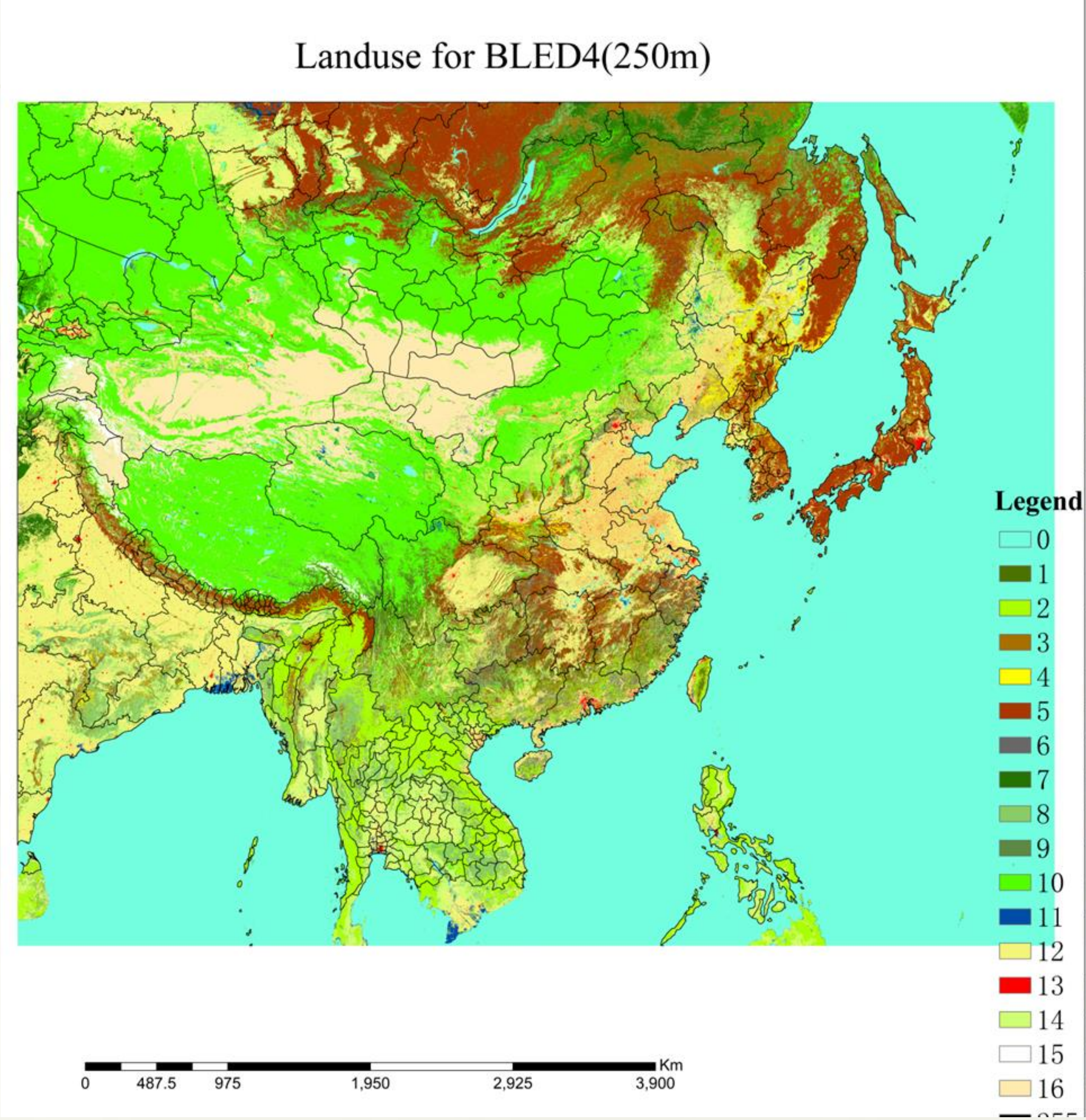
Source: FEST-C UNC-chapel hill

Three main parts of the system

- Landcover and crop categories
- Soil
- Crop management

BLED4

- Landuse
  - FORM-LC(250m) China
  - MODIS（500m） Other regions



MODIS Class Name
Water
Evergreen Needleleaf Forest
Evergreen Broadleaf Forest
Deciduous Needleleaf Forest
Deciduous Broadleaf Forest
Mixed Forests
Closed Shrublands
Open Shrublands
Woody Savannas
Savannas
Grasslands
Permanent Wetlands
Croplands
Urban and Built Up
Cropland/Natural Vegetation Mosaic
Permanent Snow and Ice
Barren or Sparsely Vegetated
IGBP Water
Unclassified

BLED4

- Grid crop data

Table 1. The 42 rain-fed and irrigated crops modeled in the FEST-C system.

BELD4	BELD3	Crop Name	BELD4	BELD3	Crop Name	BELD4	BELD3	Crop Name
1	22	Hay	15	36	Cotton	29	50	SorghumSilage
2	23	Hay_ir	16	37	Cotton_ir	30	51	SorghumSilage_ir
3	24	Alfalfa	17	38	Oats	31	52	Soybeans
4	25	Alfalfa_ir	18	39	Oats_ir	32	53	Soybeans_ir
5	26	Other_Grass	19	40	Peanuts	33	54	Wheat_Spring
6	27	Other_Grass_ir	20	41	Peanuts_ir	34	55	Wheat_Spring_ir
7	28	Barley	21	42	Potatoes	35	56	Wheat_Winter
8	29	Barley_ir	22	43	Potatoes_ir	36	57	Wheat_Winter_ir
9	30	BeansEdible	23	44	Rice	37	58	Other_Crop
10	31	BeansEdible_ir	24	45	Rice_ir	38	59	Other_Crop_ir
11	32	CornGrain	25	46	Rye	39	60	Canola
12	33	CornGrain_ir	26	47	Rye_ir	40	61	Canola_ir
13	34	CornSilage	27	48	SorghumGrain	41	62	Beans
14	35	CornSilage_ir	28	49	SorghumGrain_ir	42	63	Beans_ir

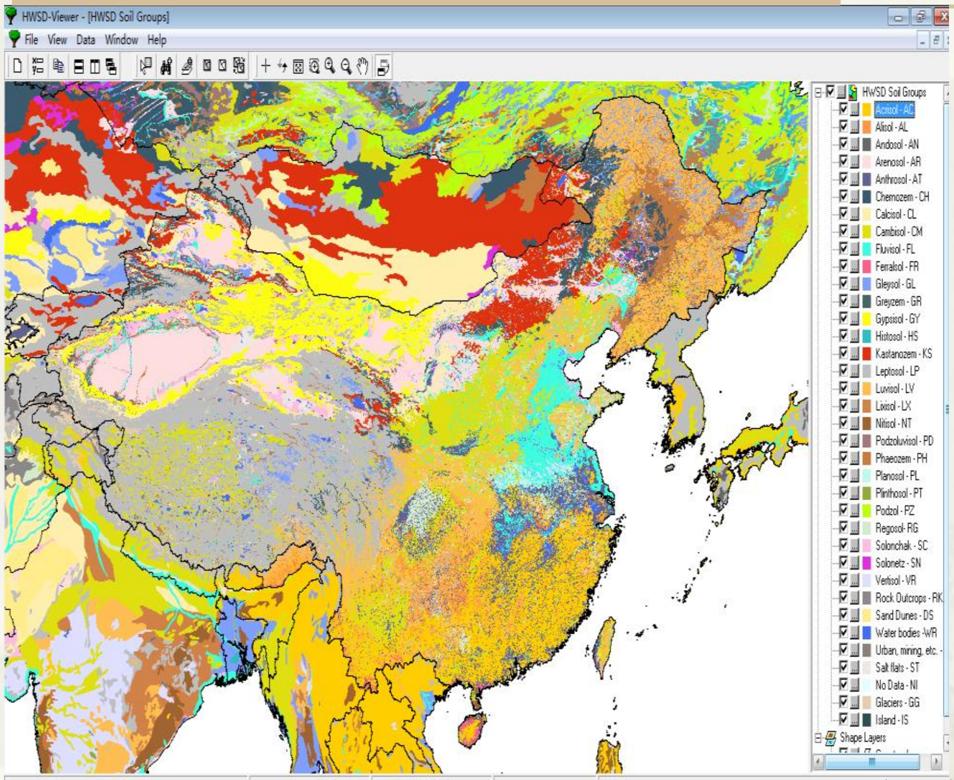
- 15 crop categories: including early rice, middle rice, late rice, winter wheat, spring wheat, corn, sorghum, barley, soybean, potato, peanuts, canola, cotton and other crops , Pasture
- Each crop is divided into irrigated and non-irrigated classes, so we’ll have 30 rain-fed and irrigated crops modeled in FEST-C system.

Soil map （main part）

- HWSD soil data set will be used for China EPIC soil, but the data is a little rough. Resolution is 36km . The data is provided from the Institute of Soil Science, Chinese Academy of Sciences, China
- 1.There is only two soil layers from HWSD :- top layer (0-30cm);sub layer (30-100cm).
- 2. Lack essential elements like : soil albedo, Initial soil water content, fraction of field capacity, groundwater storage in mm …

Generating Site Soil Data

Harmonized World Soil Dataset (1km * 1km)



Variable	Units	China
Gravel Content	%vol.	√
Sand Fraction	% wt.	√
Silt Fraction	% wt.	√
Clay Fraction	% wt.	√
Texture Classification	name	√
Reference Bulk Density	kg/dm3	√
Bulk Density	kg/dm3	√
Organic Carbon	% weight	√
pH (H2O)	-log(H+)	√
CEC	Cmol/kg	√
Base Saturation	%	√
……………………		

Soil input file for 36km each grid

Generating Grid Crop Data

line 1: (columns 1-n)

General description line for soil type.

line 2: (fields of 8 columns)

2	SALB	=	soil albedo.
3	HSG	=	soil hydrologic group (1=A, 2=B, 3=C, 4=D).
4	FFC	=	Initial soil water content, fraction of field capa
5	WTMN	=	min depth to water table in m, (blank if unknov
6	WTMX	=	max depth to water table in m, (blank if unkno
7	WTBL	=	initial water table height in m, (blank if unknov
8	GWST	=	groundwater storage in mm (blank if unknown
9	GWMX	=	maximum groundwater storage in mm (blank i
10	RFT0	=	groundwater residence time in days, (blank if u
11	RFPK	=	return flow/(return flow + deep percolation), (t

line 3: (fields of 8 columns)

12	TSLA	=	maximum number of soil layers after splitting
		=	0 no splitting occurs initially.
13	XIDP	=	soil weathering code.
		=	0 for calcareous and non-calcareous soils with
		=	1 for non CACO3 slightly weathered.
		=	2 for non CACO3 moderately weathered.
		=	3 for non CACO3 highly weathered.
		=	4 input PSP or active + stable mineral P (kg/h
14	RTN0	=	number of years of cultivation at start of simul
15	XIDK	=	1 for kaolinitic soil group.
		=	2 for mixed soil group.
		=	3 for smectitic soil group.
16	ZQT	=	minimum thickness of maximum layer (M) (splitting stops when ZQT is reached).
17	ZF	=	minimum profile thickness (M) – stops simula
18	ZTK	=	minimum layer thickness for beginning simula splitting – model splits first layer with thicknes exists the thickest layer is split.
19	FBM	=	Fraction of Org C in biomass Pool (0.03 – 0.0
20	FHP	=	Fraction of Org C in passive Pool (0.3 – 0.7)

from **line 4** onward, one column of data per soil layer (up to 10 layers) (fields of 8 columns)

line 4:	Z	=	Depth to bottom of layer (M)
line 5:	BD	=	Bulk Density (T/M**3)
line 6:	UW	=	Soil water content at wilting point (1500 KPA) (M/M) (blank if unknown).
line 7:	FC	=	Water content at field capacity (33 KPA) (M/M) (blank if unknown).
line 8:	SAN	=	% sand.
line 9:	SIL	=	% silt.
line 10:	WN	=	Initial organic N Concentration (G/T) (blank if unknown).
line 11:	PH	=	soil PH.
line 12:	SMB	=	sum of BASES (CMOL/KG) (blank if unknown).
line 13:	WOC	=	organic carbon concentration (%).
line 14:	CAC	=	Calcium carbonate content of soil (%), (blank if unknown).
line 15:	CEC	=	Cation exchange capacity (cmol/kg), (blank if unknown).
line 16:	ROK	=	Coarse fragment content (% vol), (blank if unknown).
line 17:	CNDS	=	Initial NO3 concentration (G/T), (blank if unknown).
line 18:	PKRZ	=	Initial labile P concentration (1) (g/t), (blank if unknown).
line 19:	RSD	=	Crop residue (t/ha), (blank if unknown).
line 20:	BDD	=	Bulk density (oven dry) (t/m**3).
line 21:	PSP	=	<= 1 Phosphorus sorption ratio > 1 Active & stable mineral P (kg/ha)
line 22:	SATC	=	Saturated conductivity (mm/h).
line 23:	HCL	=	Lateral hydraulic conductivity (mm/h), (blank if unknown).
line 24:	WPO	=	Initial organic P concentration (g/t), (blank if unknown).
line 25:	EXCK	=	Exchangeable K concentration (g/t)
line 26 :	ECND	=	Electrical condition (mmho/cm)
line 27 :	STFR	=	Fraction of storage interacting with NO3 leaching (blank if unknown)
line 28:	ST	=	Initial soil water storage (fraction of field capacity)
line 29:	CPRV	=	Fraction inflow partitioned to vertical crack or pipe flow (blank if unknown).
line 30:	CPRH	=	Fraction inflow partitioned to horizontal crack or pipe flow (blank if unknown).
line 31:	WLS	=	Structural litter (kg/ha)
line 32:	WLM	=	Metabolic litter (kg/ha)
line 33:	WLSL	=	Lignin content of structural litter (kg/ha) (BUI)
line 34:	WLSC	=	Carbon content of structural litter (kg/ha) (BUI)
line 35:	WLMC	=	Carbon content of metabolic litter (kg/ha) (BUI)
line 36:	WLSLC	=	Carbon content of lignin of structural litter (kg/ha) (BUI)
line 37:	WLSLNC	=	N content of lignin of structural litter (kg/ha) (BUI)
line 38:	WBMC	=	Carbon content of biomass (kg/ha) (BUI)
line 39:	WHSC	=	Carbon content of slow humus (kg/ha) (BUI)
line 40:	WHPC	=	Carbon content of passive humus (kg/ha) (BUI)
line 41:	WLSN	=	N content of structural litter (kg/ha) (BUI)
line 42:	WLMN	=	N content of metabolic litter (kg/ha) (BUI)
line 43:	WBMN	=	N content of biomass (kg/ha) (BUI)
line 44:	WHSN	=	N content of slow humus (kg/ha) (BUI)
line 45:	WHPN	=	N content of passive humus (kg/ha) (BUI)
line 46:	OBC	=	Observed Carbon content at end of simulation (t/ha)

Soil files

Baumer(U.S.A)

```
 10001TX0038TXC.SOL  SINTON                                    33A1      SCL     0    1
MUSHACU    9634 2 6 2    B    2  0.05
     0.05     2.00     0.00     1.82     0.00     0.00     0.00     0.00     0.00
0.00
    10.00     2.00   100.00     2.00     0.10     0.10     1.00     0.04     0.50
     0.10     0.20     0.86     1.64
     1.48     1.48     1.48     1.52
     0.17     0.17     0.17     0.14
     0.33     0.33     0.33     0.25
    55.08    55.08    55.08    59.48
    17.42    17.42    17.42    18.02
     0.00     0.00     0.00     0.00
     6.60     6.60     7.90     7.90
     0.00     0.00     0.00     0.00
     1.56     1.33     0.33     0.05
    15.00    15.00    15.00    17.50
    22.50    22.50    22.50    22.50
     1.12     1.12     1.12     1.16
     5.00     5.00     5.00     2.00
     8.00     8.00     8.00     4.00
     0.00     0.00     0.00     0.00
     1.54     1.54     1.54     1.57
     0.00     0.00     0.00     0.00
    27.83    27.83    27.83    87.54
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
     0.00     0.00     0.00     0.00
```

HWSD（china）

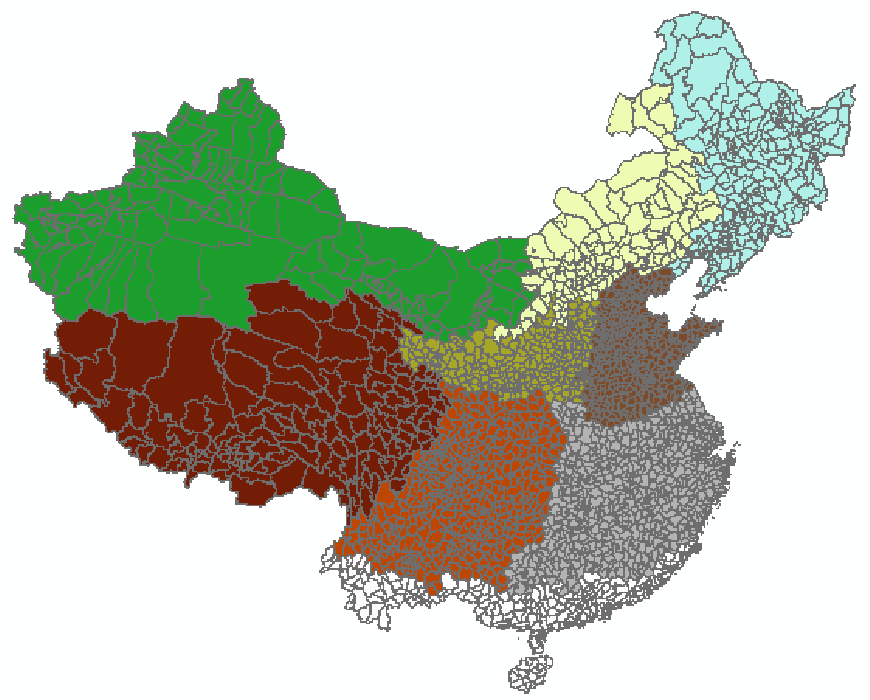
```
HWSD4636KM.SOL    GRIDID    46   3690     4     2   CM
  0.05   2.00   0.00   1.82   0.00   0.00   0.00   0.00   0.00   0.00
  2.00   3.00 200.00   2.00   0.10   0.10   1.00   0.02   0.30
  0.30   0.70
  1.31   1.30
  0.00   0.00
  0.00   0.00
 52.00  48.00
 25.00  24.00
  0.00   0.00
  4.70   4.90
  0.00   0.00
  0.95   0.35
  0.00   0.00
  6.00   5.00
  0.00   0.00
  0.00   0.00
  0.00   0.00
  0.00   0.00
  1.41   1.37
  0.00   0.00
 27.78   0.28
```

Crop management :Fertilizer application data

Application ratio of N for different fertilizer types, crops, timing and provinces

Ratio of basal fertilizer and topdressing fertilizer for different fertilizer types, crops and agriculture regions

This data is mainly based on Chinese literatures, and also refers to US case.

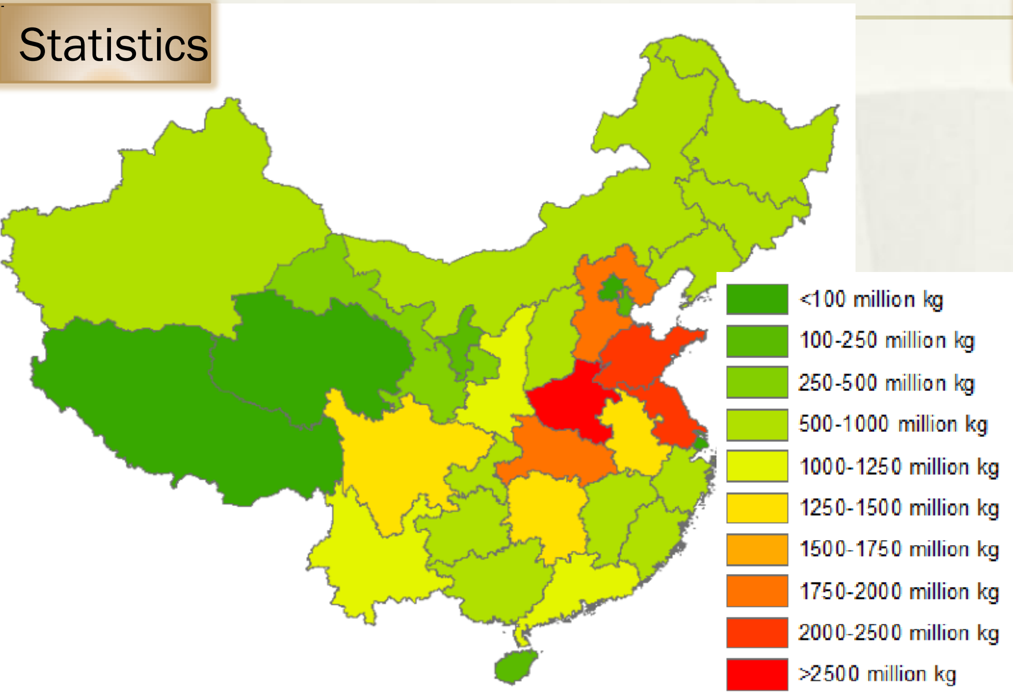


Application amount for different fertilizer types, crops and provinces

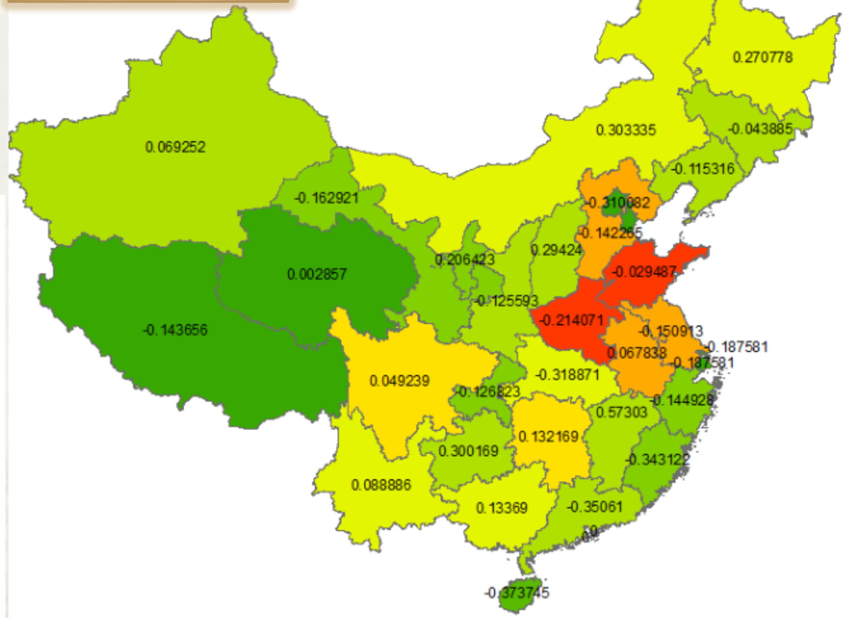
The major fertilizers containing N in China are urea and ammonium bicarbonate (total about 80-90%) , DAP ……

EPIC Output — annual fertilizer use

Statistics



EPIC output



The EPIC output can generally catch the pattern of fertilizer use from statistics data. The bias for Henan, Shandong and Jiangsu are -21%, -3% and -15%, respectively.

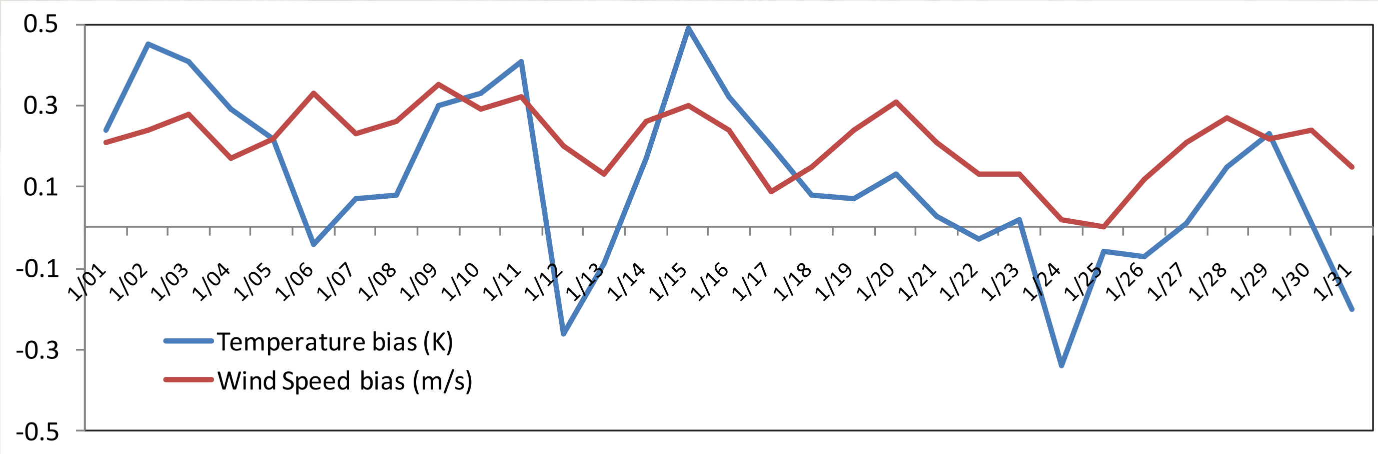
- Tillage: still working on

Generating Site Weather Data

- Weather data of 20 or 30 years should be processed for EPIC spin-up simulations to generate soil files and initial annual plant N demand data, which are used in EPIC application year simulations.

  NASA Modern Era Reanalysis for Research and Applications (MERRA) (1979-2010, 0.5° x 0.667°)

- **Generating site weather data for application year from WRF output.**



WRF evaluation

CMAQ Simulation

- Simulations using CMAQ v5.0.1
  - June and November in 2011 simulations
- Two model cases were simulated

Base case

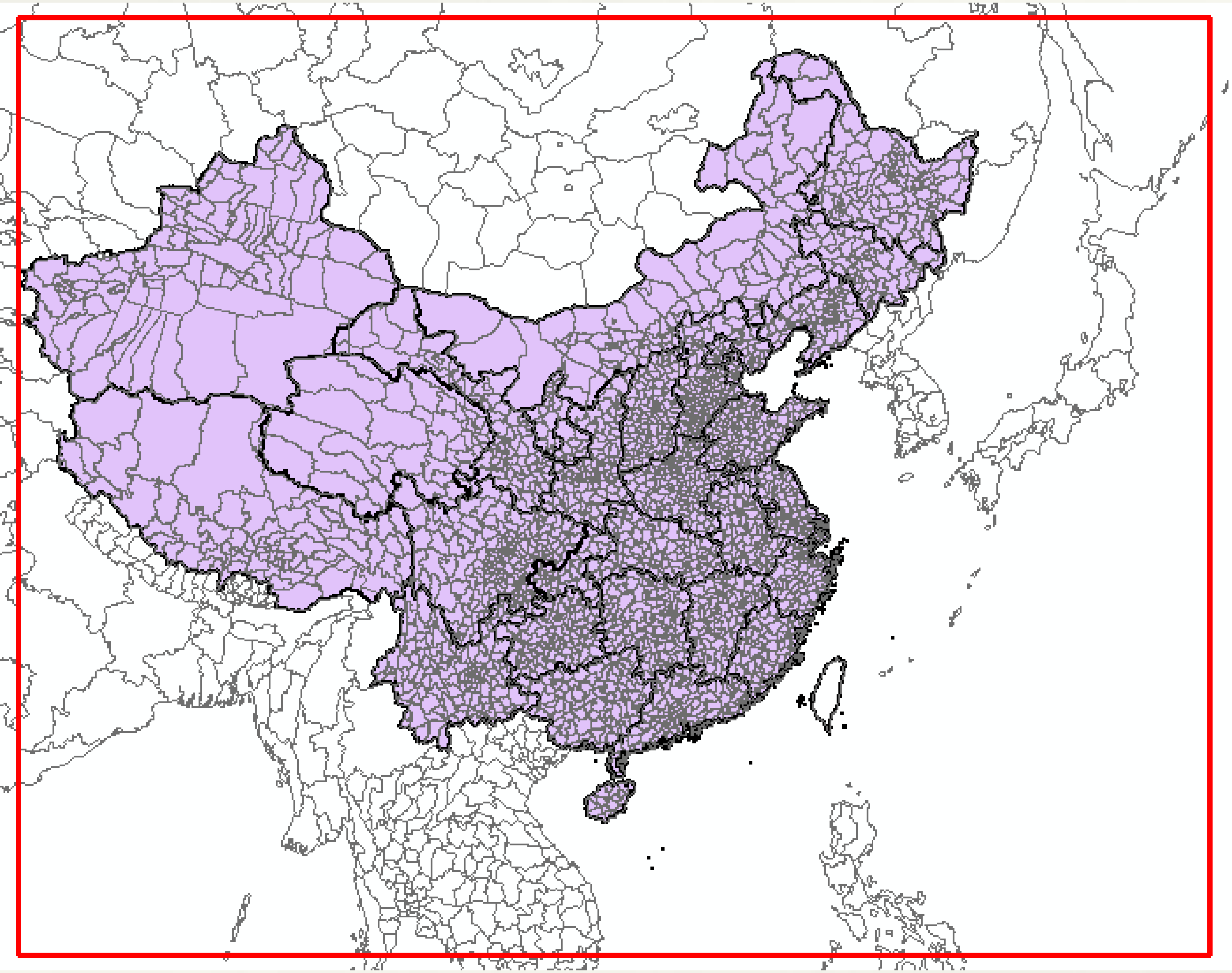
  - Emissions inventory from Tsinghua University
  - No bidirectional NH_3 exchange

Bidi case

  - Emissions inventory from Tsinghua University without NH_3 evasion from agricultural cropping sectors + FESTC NH_3 emission
  - Bidirectional NH_3 exchange

Identical model inputs and configurations except for the NH_3 emissions from cropping systems and bidirectional NH_3 exchange

The Object Domain



Target Area

–The Whole China

Target Year

–2011

Horizontal Resolution:

–36km×36km;

Future work

- Collect the tillage data of the nine agriculture regions in China (under going)
- The whole year simulation
- Further evaluating the model results and estimate the impact of major agricultural emission on $PM_{2.5}$ and future air quality
- Further applying this system (e.g. climate change, livestock)

Thank you !