11th Better Air Quality Conference (BAQ)

Development and Application of the Global Nested Air Quality Prediction Modeling System (GNAQPMS) for Mitigating Air Pollution in PR China

Zifa Wang

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The overall situation of $PM_{2.5}$ and O_3 pollution in cities and key regions over PR China

Tendency：

- $PM_{2.5}$： **sharp** reduction
- NO_2 : slow reduction
- O_3 : fluctuant increase

Degree ：

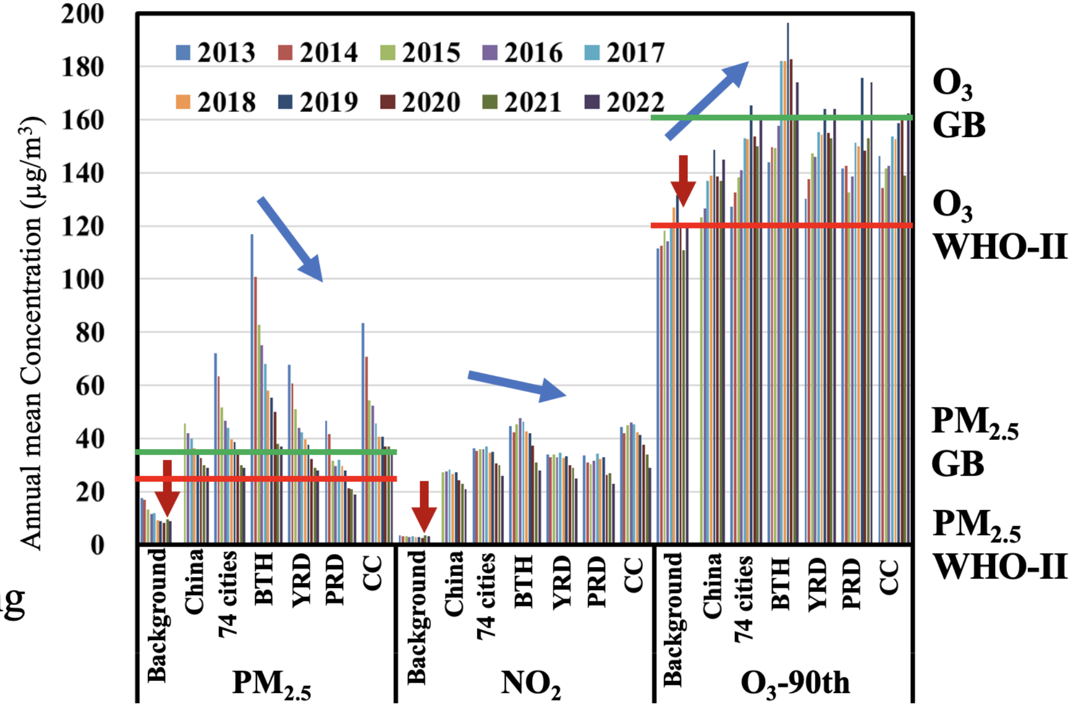
- Urban >> Background

BTH： Beijing/Tianjin/Hebei

YRD： Shanghai/Jiangsu/Zhejiang

PRD: the Pearl Delta region

CC: Chongqing/Sichuan



Evolution of annual evaluation indicators of major pollutants from 2013 to 2022

(Zhang YH, 2023)

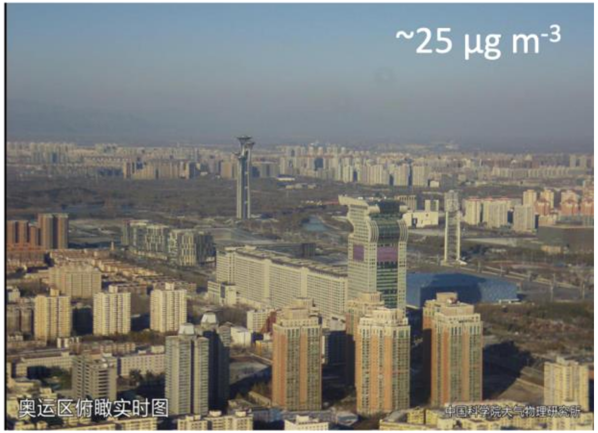
Great Needs of Accurate Prediction in PR China

- China's air pollution problem has NOT been fundamentally resolved.
- Scientific understanding on air pollution need to be refined further.

Air pollution still occurred during the COVID-19 control period. What was the source of pollution? How did it occur?

Polluted Day

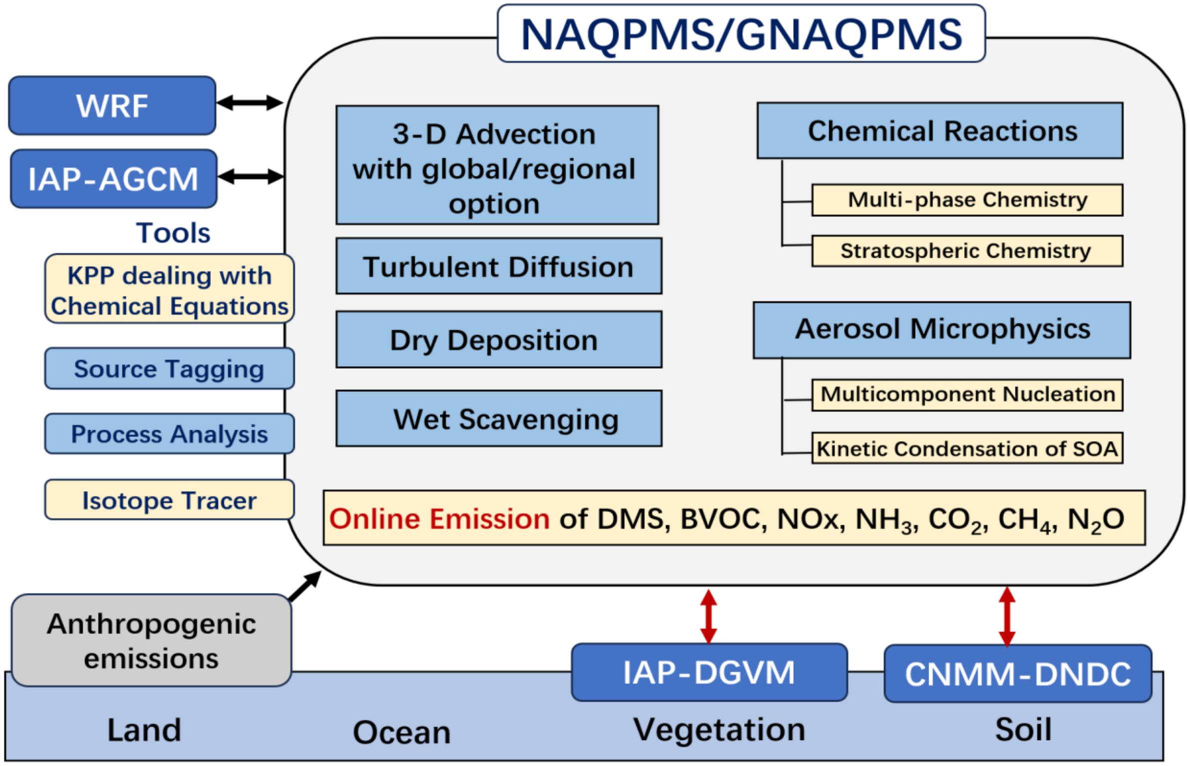
Clean Day



The performance of model is NOT good in some cases.

How to improve?

Unified framework of NAQPMS/GNAQPMS



- **Air quality forecasting**
- **Source investigation**
- **Cycle of trace species**
- **Evaluating health risks**
- **Quantifying climate forcing**

JAC 2006; JGR, 2007; ACP 2013; SOLA 2012； GRL 2009； AE 2011; Tellus –B 2013； ACP 2014;EP 2014; AE 2014; SC 2014;ACP 2016; AE 2017; EP 2017; GMD, 2015; SOLA, 2014; EP, 2017, AE,2019; ACP, 2019, 2021; GMD, 2021; AE, 2021; ACP, 2023; GMD,2023

New updates in physical and chemical schemes

Advancing the model ability and representation of model processes

① Gas and heterogeneous chemistry

② Secondary organic aerosol module

③ Online emission of BVOC and DMS

④ Aerosol microphysical processes

⑤ Isotope simulation and tracing

⑥ Stratospheric chemistry

Incorporating KPP to resolve chemical kinetic systems

Facilitating GNAQPMS to update scheme and increase new reactions

- Edit equation files
- KPP generates code
- Coupling interface

KPP

- Macro definition
- Compiling options
- Matching species

Simplest scheme	Medium scheme	Detailed scheme
Long-term simulation	Short-term coupled simulation	Episode simulation

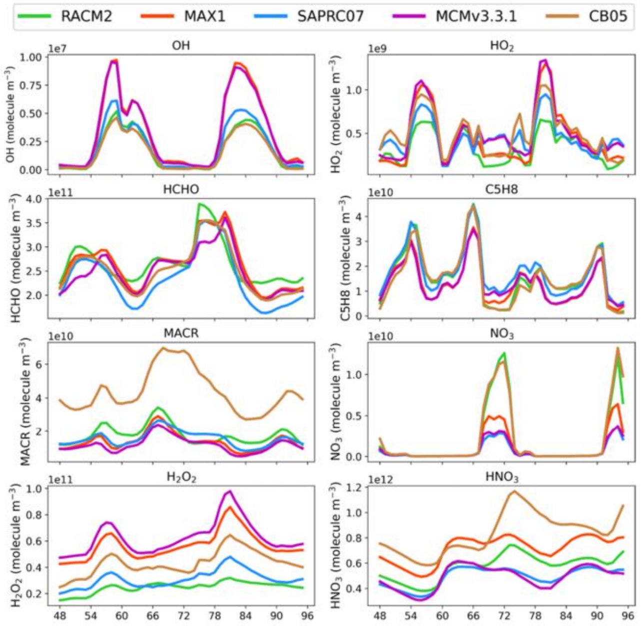
Develop atmospheric chemical mechanism MAX1 in PR China

- ✓ Organic peroxyradicals (RO2, RCO3, etc.) and Kirchner radicals (RCHOO)
- ✓ Hydrogen transfer reactions

Comparison MAX1 with other mechanisms

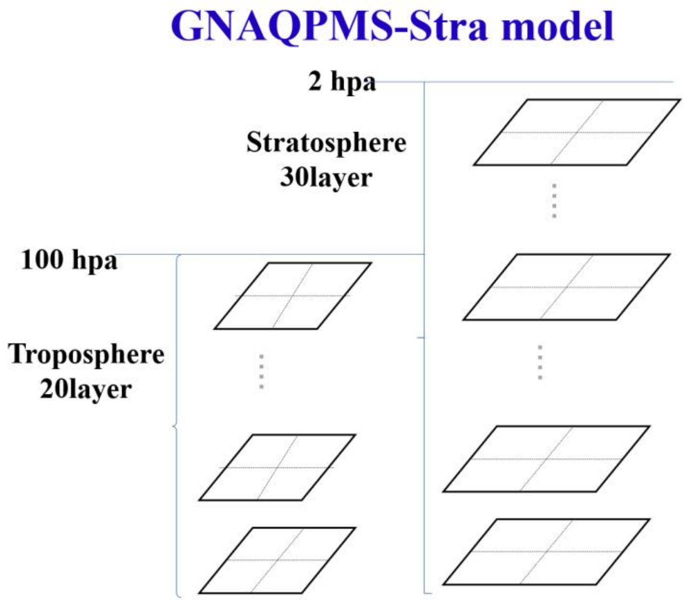
mechanism	version	type	Inorganic reaction number
RADM	RADM2	condensed	38
Carbon Bond	CB05	condensed	54
MOZART	MOZART-4	condensed	46
SAPRC	SAPRC07	condensed	55
RACM	RACM2	condensed	46
MCM	MCM3.3.1	near-explicit	45
MAX1	**MAX1**	**condensed**	**60**

MAX1 has good performance



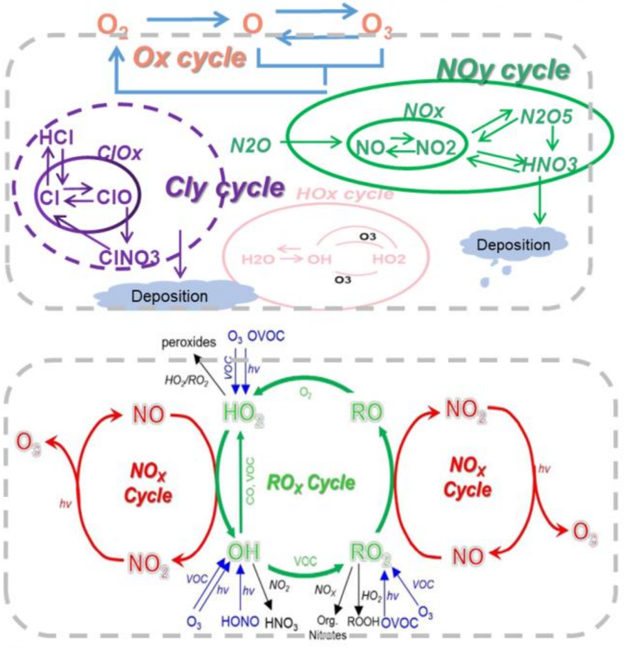
Develop tropospheric chemistry using KPP in GNAQPMS

Meteorological model: GWRF, 0.5º resolution
Height: Surface-2 hpa, 50 layers；
Chemistry: 115 species, 262 reactions



Zhang et al., ERL, 2023

Stratospheric chemistry (O_x-NO_x-HO_x-BrO_x-ClO_x)

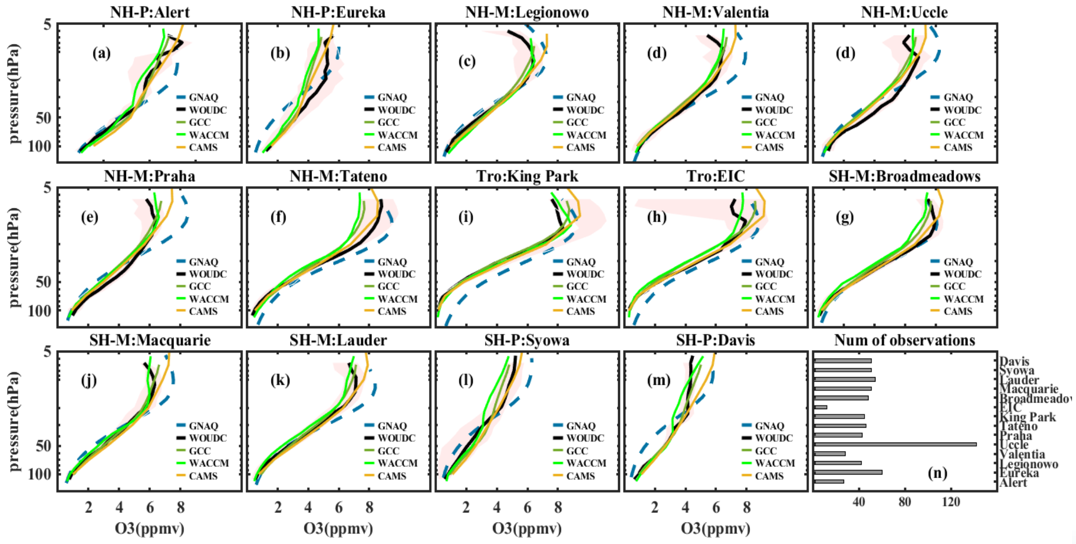


Tropospheric chemistry(NOx-VOC-CO)

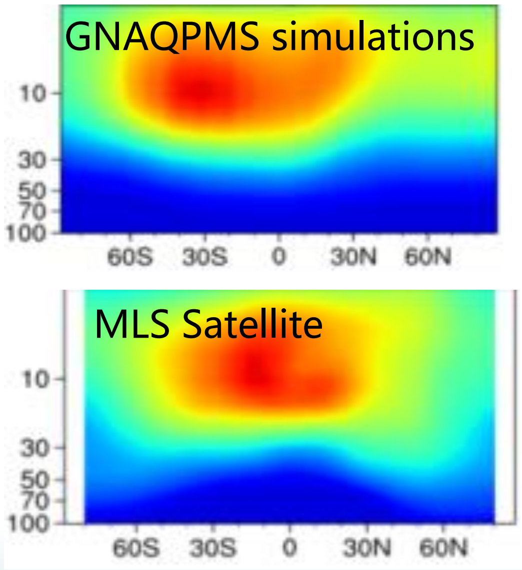
GNAQPMS has good skills in simulating stratospheric O_3

✓ Model reproduced observed ozone profiles in the stratosphere

Comparison with WOUDC ozonesonde observations



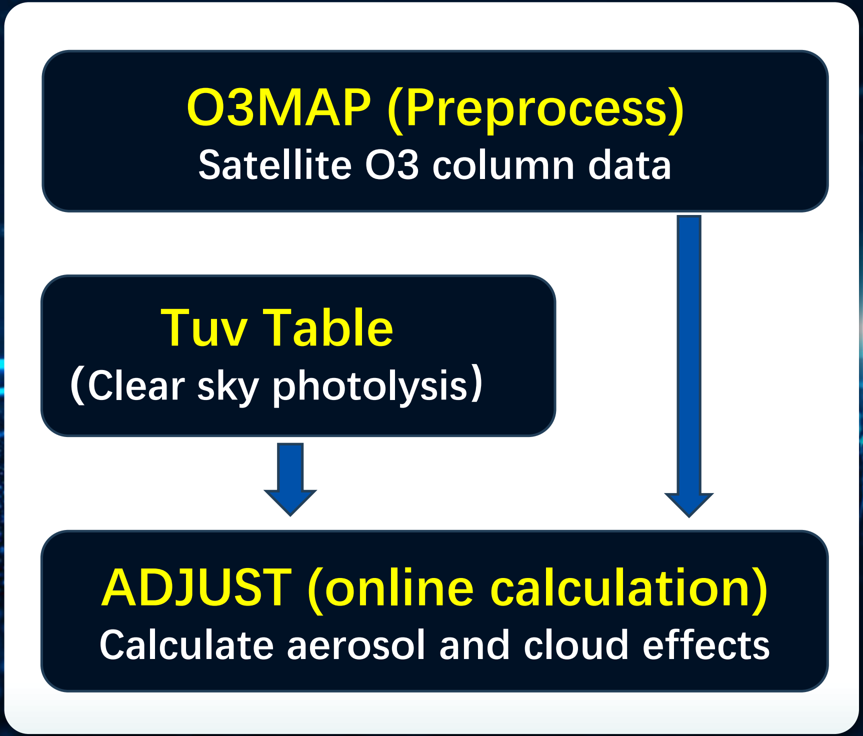
Zonal and vertical distributions of stratospheric ozone



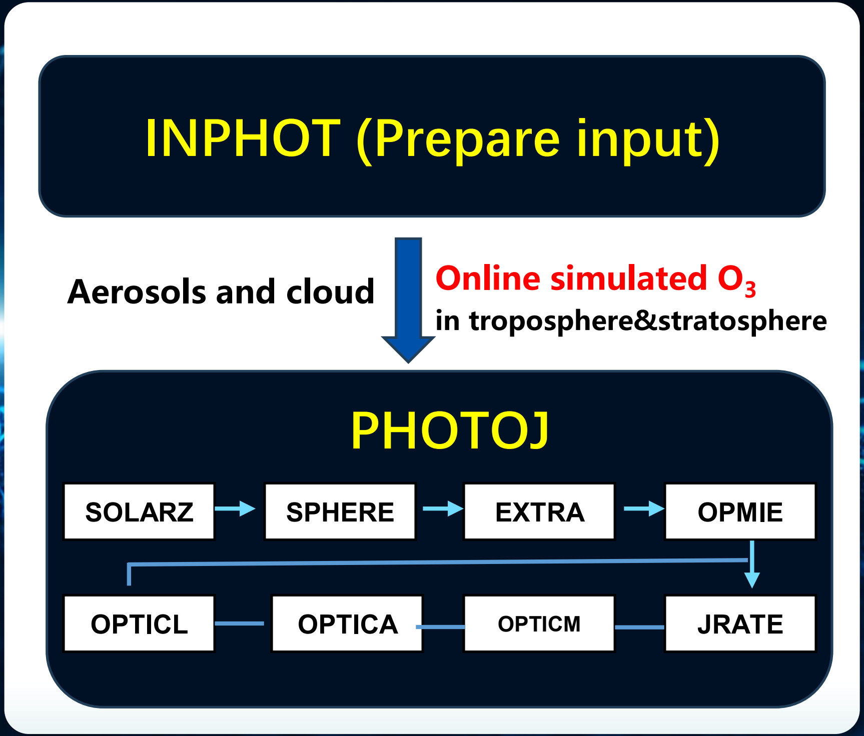
Zhang et al., 2023

Incorporating two schemes for photolysis rate calculation

TUV for troposphere simulation



Fast-JX for troposphere&stratosphere



Consider HONO source and heterogeneous mechanism

Add new emission sources and heterogeneous reaction pathways

- **Soil emission, indoor emission, biomass burning and updated mobile emission**

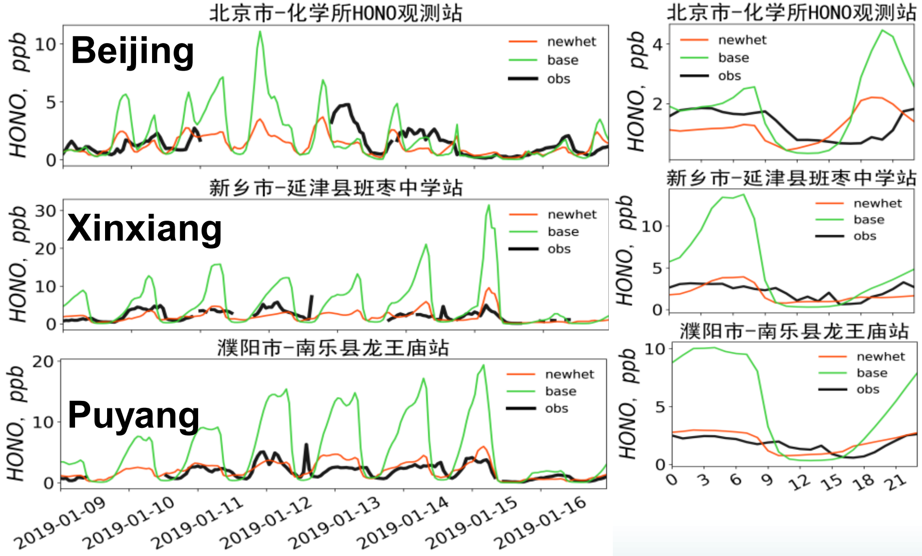
$$F_N(HONO) = F_{N,opt}(HONO) \times e^{\frac{E_a}{R}\left(\frac{1}{T_{opt}} - \frac{1}{Ts}\right)} \times f(SWC)$$

- **New heterogeneous reactions**

{200:H29} NO_2 + SGRND = HONO
{201:H30} NO_2 + PAER = 0.5 HONO
{202:H31} $AERNO_3$ + SGRND + hv = 0.67 HONO + 0.33 NO_2
{203:H32} HNO_3 + SGRND + hv = 0.67 HONO + 0.33 NO_2
{204:H33} $AERNO_3$ + hv = 0.67 HONO + 0.33 NO_2

(An et al., 2013; Zhang et al. ,2022)

The overestimation at nighttime and the underestimation of HONO at daytime were significantly improved



Incorporating sulfate heterogeneous reactions

The Mn-catalytic heterogeneous reactions increase sulfate chemical production and remarkably reduce model biases

Sulfate formation scheme in WRF-Chem

- **Gas phase**

  $SO_2 + OH + H_2O + O_2 \rightarrow H_2SO_4 + HO_2$

- **Aqueous phase**

  $HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + H_2O$

  $SO_2 + O_3 + H_2O \rightarrow SO_4^{2-} + 2H^+ + O_2$

  $SO_2 + H_2O + 0.5O_2 + Fe^{3+}/Mn^{2+} \rightarrow SO_4^{2-} + 2H^+$

  $HSO_3^- + 2NO_2 + H_2O \rightarrow SO_4^{2-} + 3H^+ + 2NO_2^-$

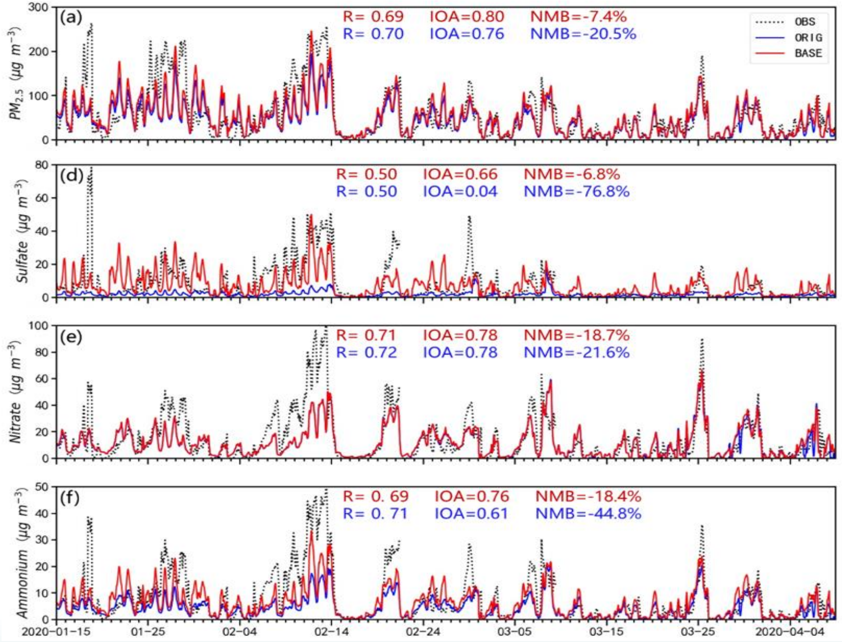
New sulfate scheme by Wang et al. (2021)

- **Transition metal-catalyzed oxidation of SO2 on aerosol surfaces**

- $SO_2 + O_2 + Mn(OH)_x^{(3-x)} \rightarrow SO_5^{\cdot-} + Mn^{2+}$, x = 1, 2

  $SO_5^{\cdot-} + Mn^{2+} + H^+ \rightarrow Mn(OH)_x^{(3-x)} + HSO_5^-$

  $NH_3 + HSO_5^- + SO_2 + H_2O \rightarrow NH_4^+ + SO_4^{2-}$



SOA module: incorporating VBS framework to GNAQPMS

POA aging+IVOCs greatly enhanced the SOA concentration and SOA/OA

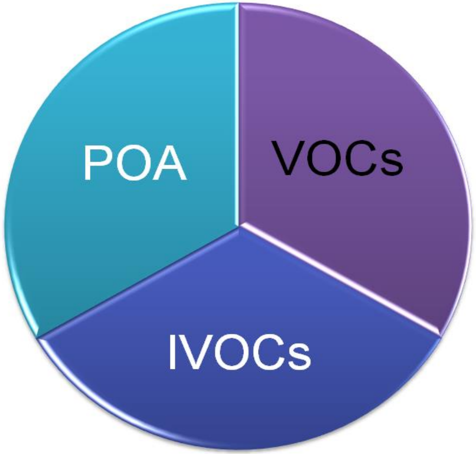
Volatility Basis Set (VBS)

↑

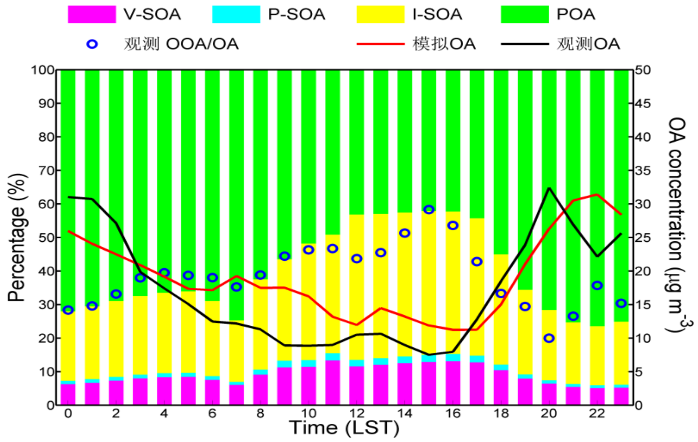
Two Product (2P)

Systematic underestimation!

(Kanakidou&Swietlicki, 2005;Lin et al., 2016)



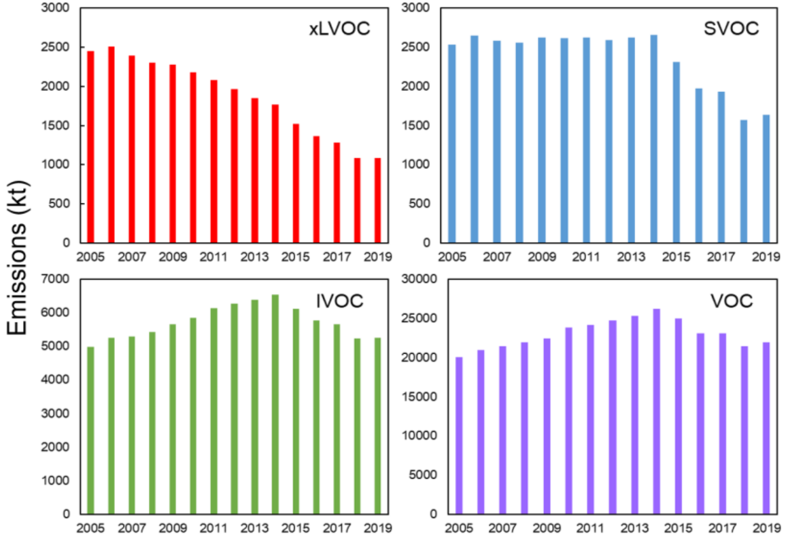
Model reproduced SOA and SOA/OA



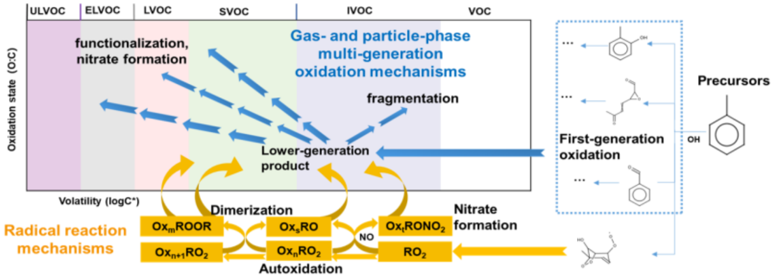
AE, 2019; ACP, 2019, 2021

Accurate source apportionment of organic aerosol by developing full-volatility organic emission inventories

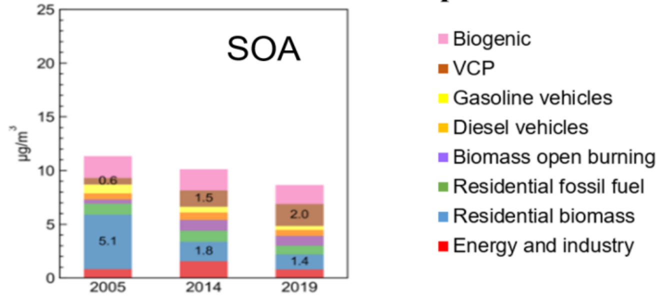
Developed the emission inventories of organics in the full volatility range for 2005-2019



Constructed the integrated two-dimensional volatility basis set (I2D-VBS) framework to systematically represent the diverse and competing organic oxidation pathways



Accurately apportioned the sources of organic aerosol in China and their temporal trend

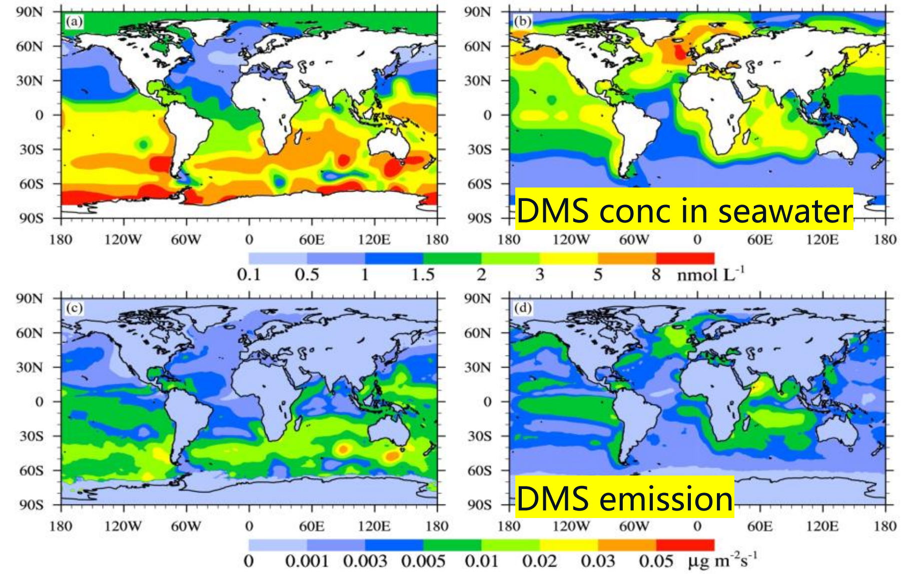


Chang X.#, Zhao B.#, …, Wang S.*, *One Earth*, 2022; Zheng H.#, Chang X.#, …, Wang S.*, *Environ Sci. Technol. Lett.*, 2023; Zheng H.#, Chang X.*, …, Wang S.*, *Environ. Sci. Technol.*, 2023

Online calculation of natural trace gases in GNAQPMS

Online emission of DMS

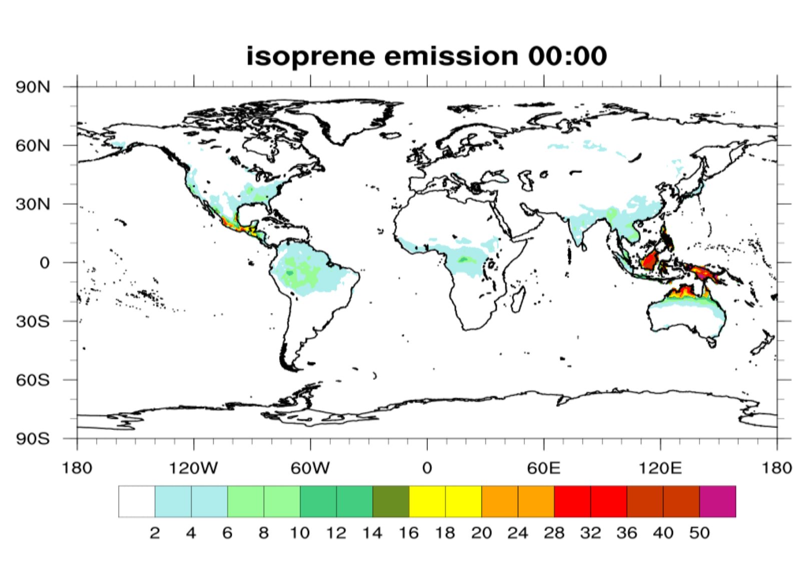
depending on seawater DMS concentration, wind, and sea surface temperature



Wei et al., ACP, 2019

Online emission of BVOCs

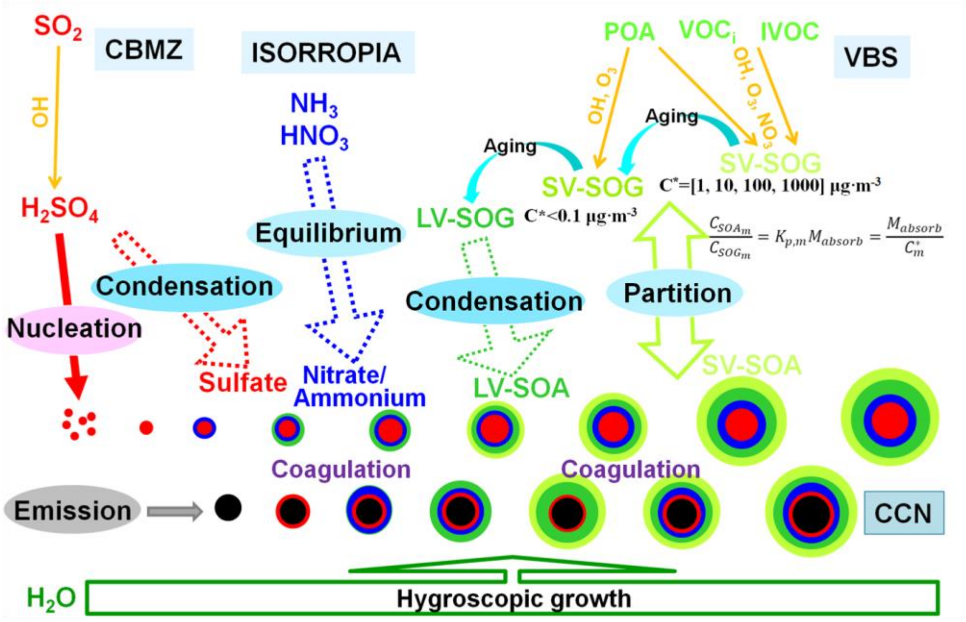
depending on vegetation and meteological factors



Yang et al., 2023 (submitted)

Advancing the modeling of aerosol microphysics

Size distribution matters more in climate effects and health risks of aerosols

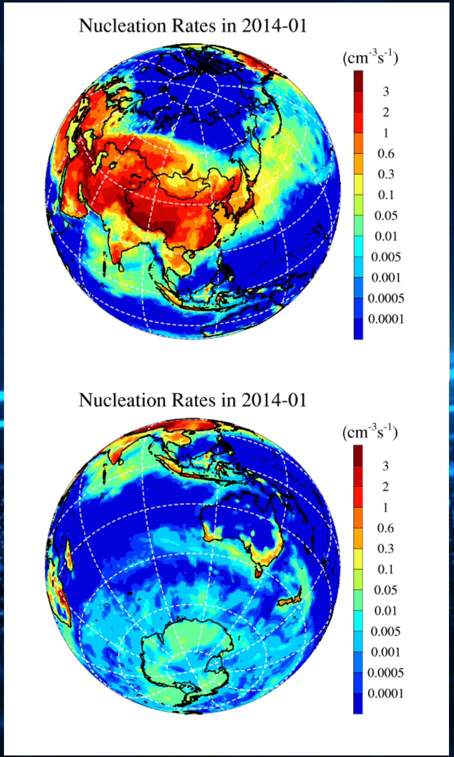


- ✓ 1nm-10μm 40 bins
- ✓ Nucleation (IMN, Org, TIMN)
- ✓ Explicit growth of new particles
- ✓ Coagulation among particles
- ✓ Aging of primary particles
- ✓ Condensation and equilibrium partition depending on volatility

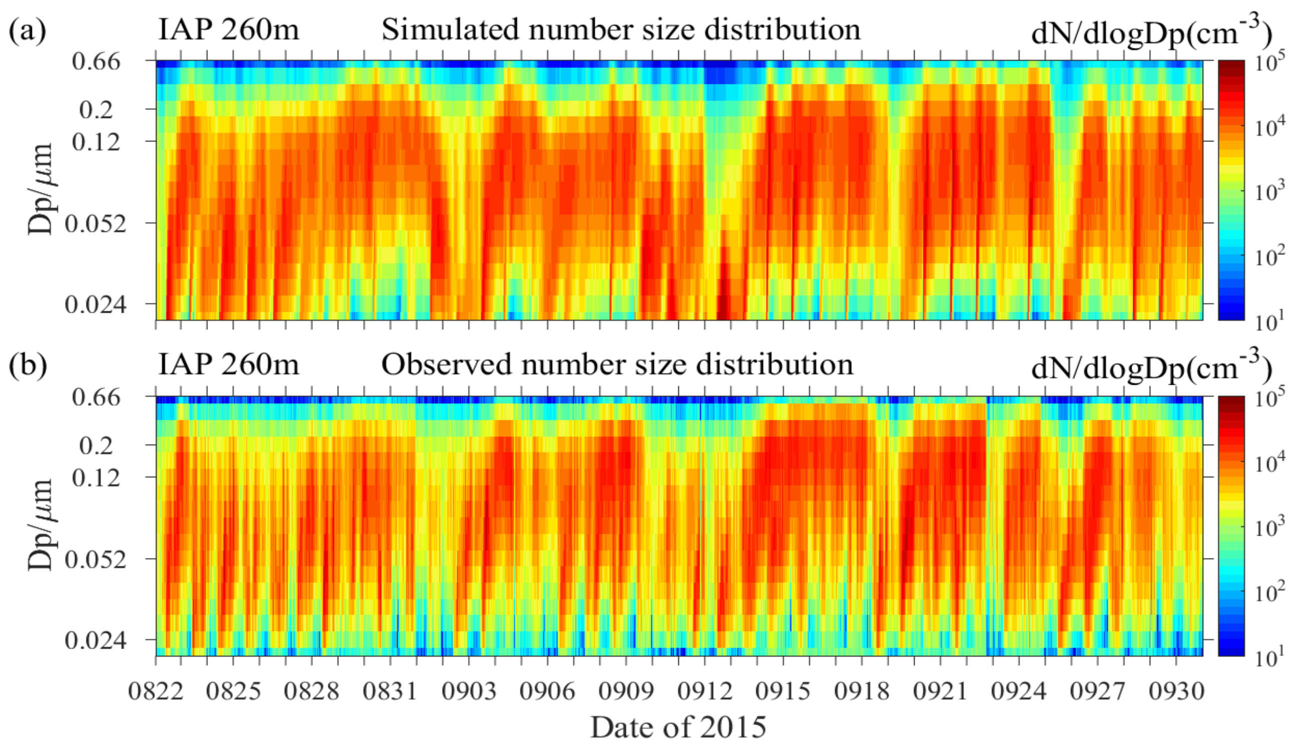
Chen et al., AE, 2019; Chen et al., ACP, 2021

GNAQPMS simulating detailed aerosol microphysical process

Nucleation rates



Reproduced the New Particle Formation events



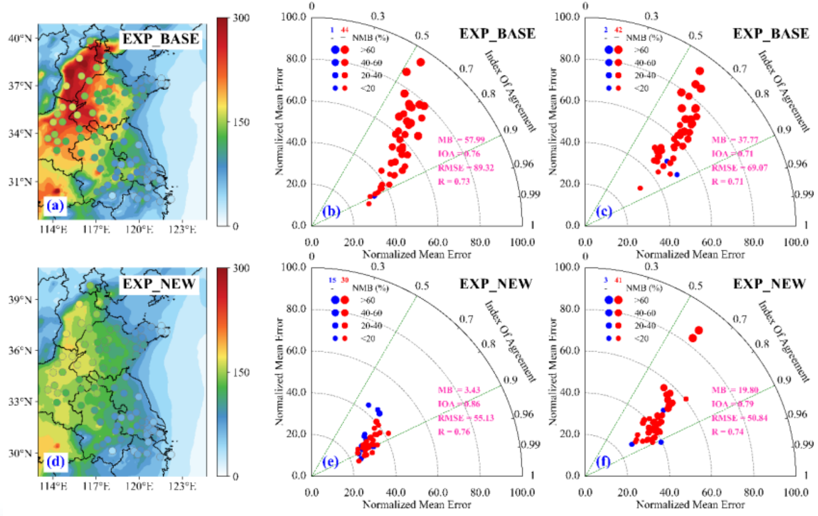
Chen et al., ACP, 2021

Parameterized minimum eddy diffusivity (Kzmin) for improving $PM_{2.5}$ simulations under stable Boundary Layer

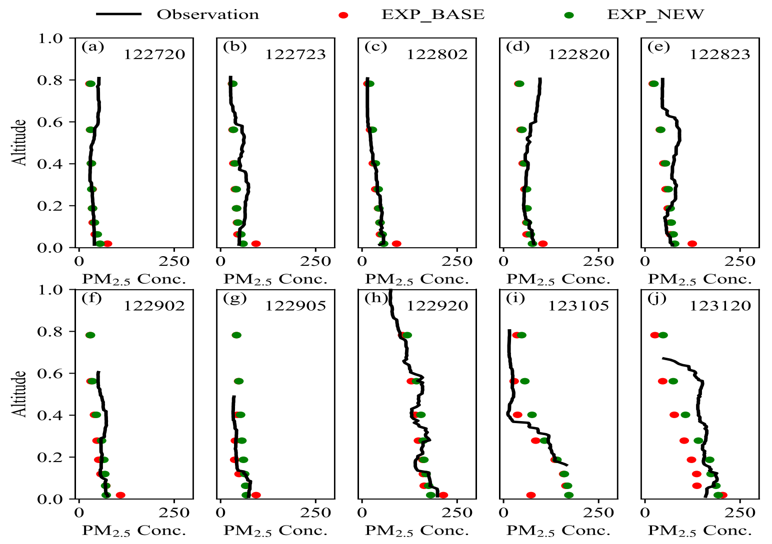
$$K_h = k w_s z \left(1 - \frac{z}{h}\right)^2 / P_r + K_{zmin}$$

$$K_{zmin} = 1 + LE/H$$

New scheme well improved $PM_{2.5}$ simulations



Improved vertical profile of $PM_{2.5}$ in BL



Lu & Zhu@GMD-discussion, 2023

Inversing emission based on ensemble Kalman filter during the COVID-19 lockdown

Inversion method: EnKF + State augmentation technique

$$x^a = x^b + \mathrm{BH}^{\mathrm{T}}\left(\mathrm{HBH}^{\mathrm{T}} + \mathrm{R}\right)^{-1}\left(y^o - \mathrm{H}x^b\right)$$

Background error **Observation error**

$$x = \begin{bmatrix} c \\ \beta \end{bmatrix} \rightarrow c = \begin{bmatrix} PM_{2.5} \\ NO_2 \\ SO_2 \\ CO \end{bmatrix} \rightarrow \beta = \begin{bmatrix} \beta_{PM_{2.5}} \\ \beta_{BC} \\ \beta_{OC} \\ \beta_{NO_x} \\ \beta_{SO_2} \\ \beta_{CO} \end{bmatrix}$$

Emission adjusting factor

Background error: Ensemble estimation with Inflation technique (Maximum likelihood estimation)

$$-2L(\lambda) = ln\left\{det\left(\mathrm{H}\lambda\mathrm{P}_{\mathrm{e}}^{\mathrm{b}}\mathrm{H}^{\mathrm{T}} + \mathrm{R}\right)\right\} + d^T\left(\mathrm{H}\lambda\mathrm{P}_{\mathrm{e}}^{\mathrm{b}}\mathrm{H}^{\mathrm{T}} + \mathrm{R}\right)^{-1}d$$

$$d = y^o - H\left(\frac{1}{N}\sum_{i=1}^{N} x_i^b\right)$$

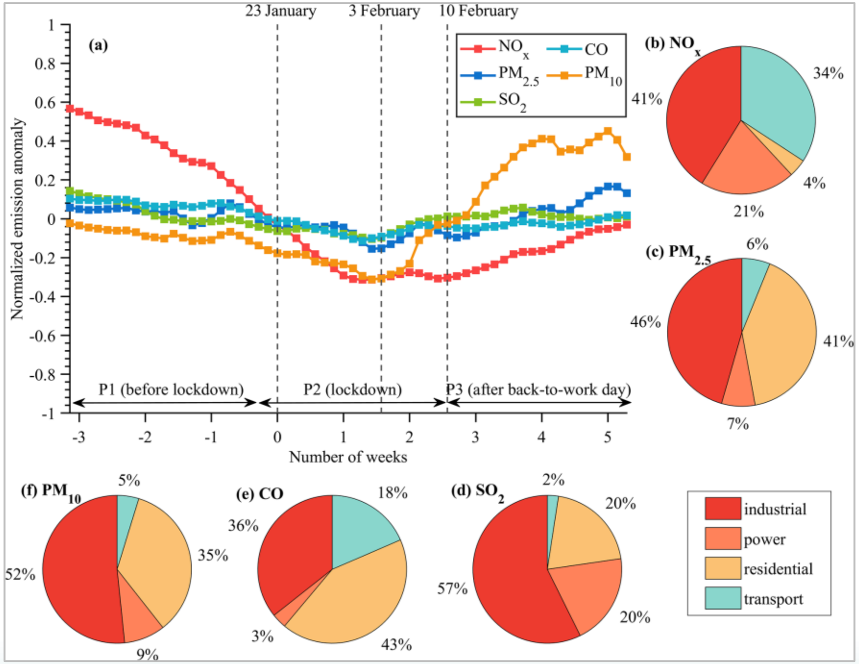
Observation error:

Measurement error ($PM_{2.5}$: 5%, SO_2, NO_2 and CO:4% (http://www.cnemc.cn/jcgf/dqhj/) + Representativeness error (Li et al., 2019)

Kong et al., ACP, 2023

Complex environmental effects of the COVID-19 lockdown

Inversed emission changes of multi-species during the lockdown



P1: Normal 2020.1.1 – 1.20.

P2: Lockdown and Spring festival 1.21 – 2.9

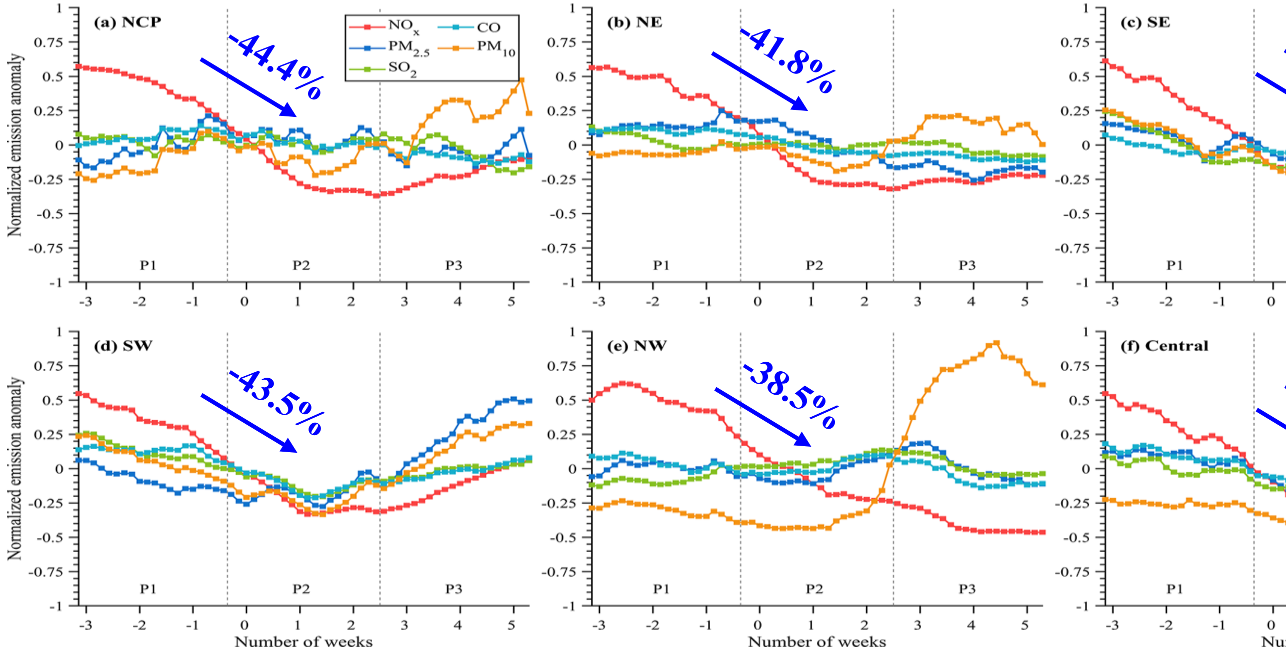
P3: Back to work 2.10 – 2.29

	NO_x	SO_2	CO	$PM_{2.5}$	PM_{10}
P1 (Gg/day)	72.9	23.8	1160.2	44.5	75.5
P2 (Gg/day)	41.9	21.5	1037.4	40.9	66.4
P3 (Gg/day)	44.8	23.2	1078.2	45.9	108.4
(P2-P1)/P1	-42.5%	-9.7%	-10.6%	-7.9%	-12.1%
(P3-P1)/P1	-38.6%	-2.5%	-7.0%	3.3%	43.6%

Kong et al., ACP, 2023

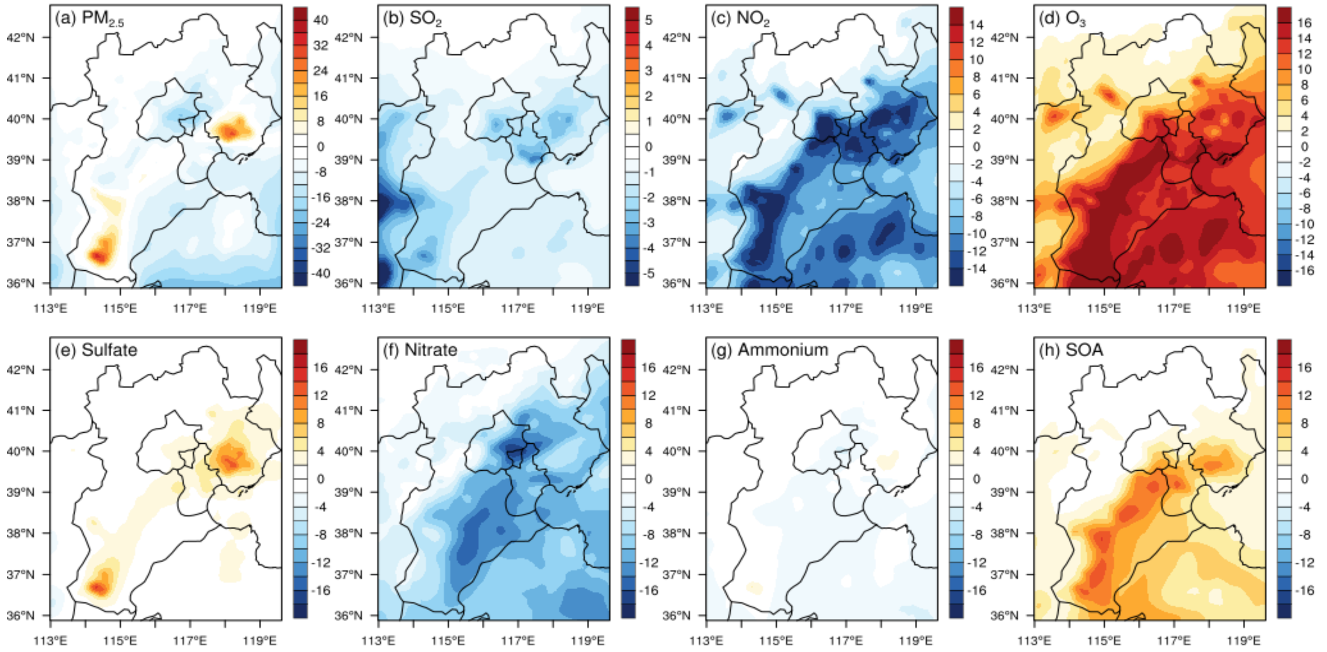
Complex environmental effects of the COVID-19 lockdown

Inversed emission changes during the lockdown



North China Plain (NCP), northeast China (NE), southeast China (SE), southwest China (SW), northwest China (NW) and central region.

Large impacts of the COVID-19 lockdown on atmospheric oxidizing capacity and particle formation



Primary pollutants ↓

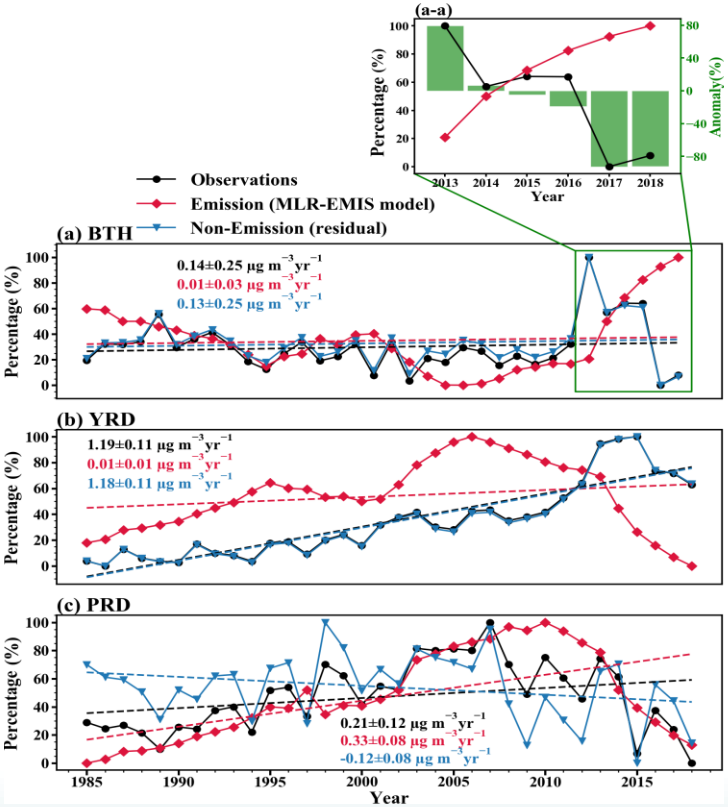
O_3 concentration ↑

Oxidizing capacity ↑

More production of secondary particles (sulfate and SOA)

Li et al., AE, 2023

Quantitative contributions of meteorology/climate to the trend of $PM_{2.5}$



- Quantitative contributions to the linear trend of $PM_{2.5}$ derived based on multiple linear regression (MLR) results alone are not credible because a good correlation in the MLR analysis does not imply any causal relationship.

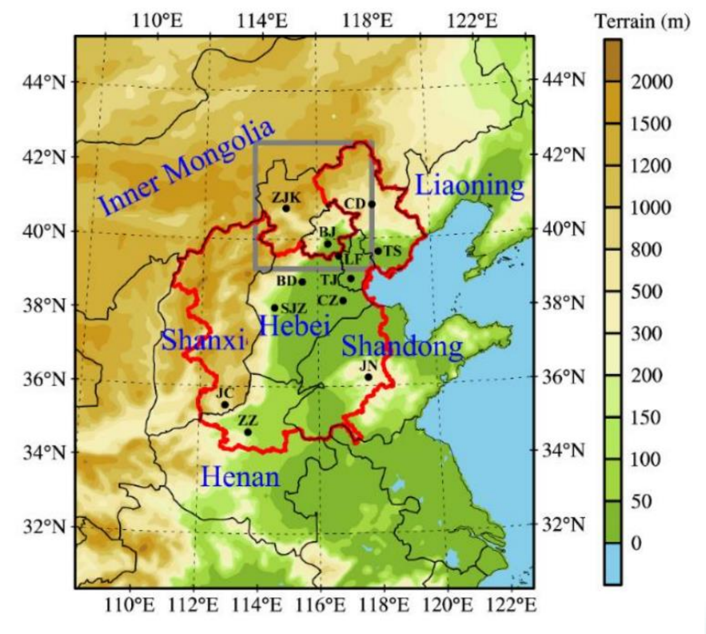
- The best estimates of the contributions of emissions and non-emission processes (including meteorology/climate) to the linear trend in $PM_{2.5}$ during 2013–2018 are :

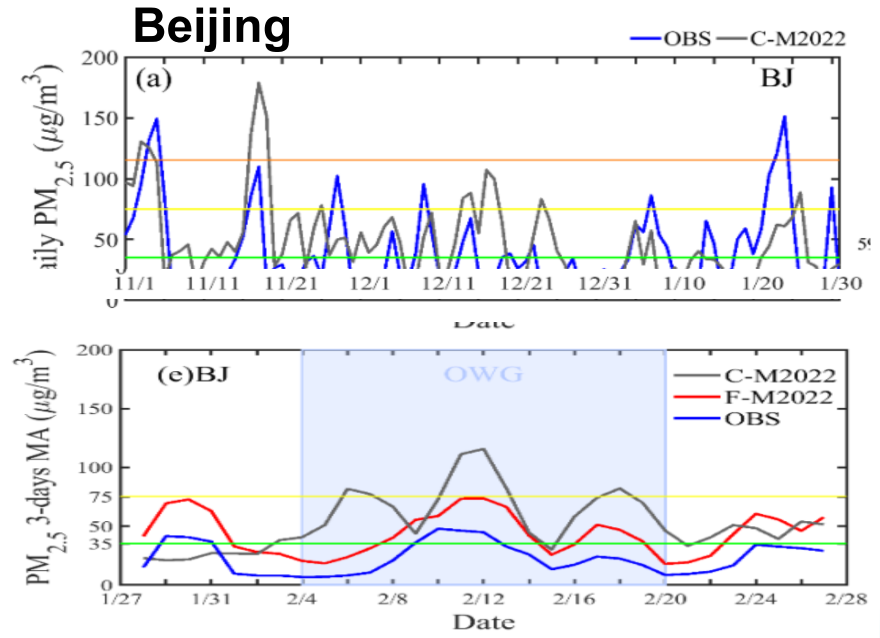
emission < 51 % and non-emission > 49 % for BTH,
emission < 44 % and non-mission > 56 % for YRD,
emission < 88 % and non-emission > 12 % for PRD.

Wu et al., ACP, 2022

Seasonal-scale predictions of air quality in the 2022 Olympic Winter Games

Model successfully predicted the trend of air quality around three months ahead the Games period, supporting emission control measures in advance





Yang et al., 2023

Accelerating GNAQPMS on Many-Integrated-Core

We present the porting and optimization of GNAQPMS on the Intel MIC, codenamed "Knights Landing" (KNL).

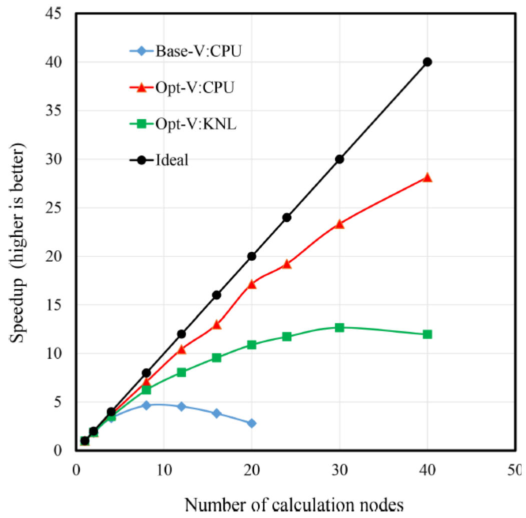


Fig. 2, Scalability of Base-V and Opt-V GNAQPMS on the CPU and KNL clusters.

CPU (E5-2697 V4 with 36 physical cores and 2 hyper-threads)				
	OMP	MPI	Wall time	Speedup
Baseline (no hyper-thread)	0	36	4381.2	1
Opt-V	1	72	1769	2.48
	2	36	1625.72	2.70
	4	18	1614.9	2.71
	6	12	1580.1	2.77
	12	6	1612.3	2.72
	18	4	1790.2	2.45
	36	2	2243.4	1.95
Opt-V (no global communication)	6	12	1623.6	2.70
KNL (KNL 7250 with 68 physical cores and 4 threads)				
Opt-V	2	136	1499.2	2.92
	4	68	1402.9	3.12
	2	68	1512.8	2.90
	4	34	1248.3	3.51
	8	34	1373.6	3.19
	16	17	1473.2	2.97
Opt-V (no global communication)	4	34	1444.6	3.03

Table 1. Speedup and wall time of different combinations of OpenMP threads and MPI processes.

The Opt-V GNAQPMS were conducted on the Xeon E5-2697V4 and KNL 7250 clusters, and achieved a speedup of **2.77 on the CPU** platform and a speedup of **3.51 on the KNL** platform in the single node.

Wang et al., GMD, 2017; Wang et al., GMD, 2019

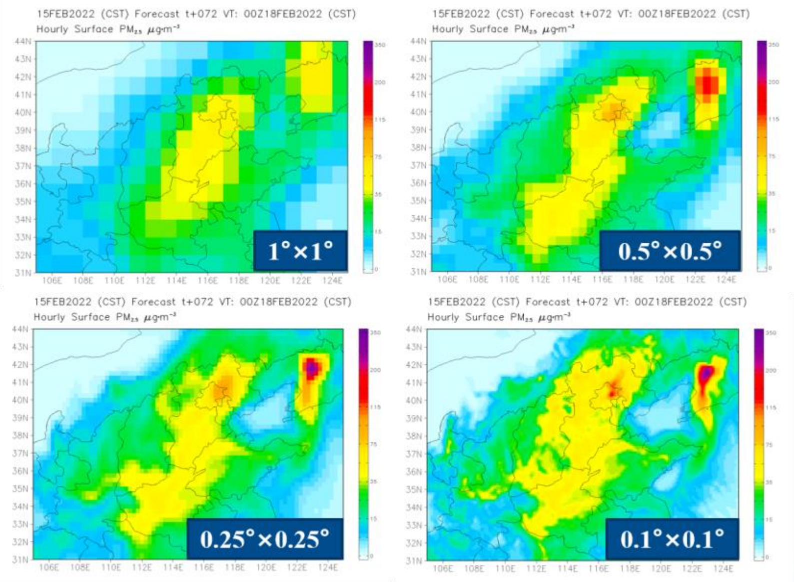
Application to global air quality forecasting

Simulation tests show that with the increase of resolution, the simulation precision increases but more HPC resources are needed

HPC computational efficiency and resource requirements for different resolutions

resolution	1x1°	0.5x0.5°	0.25x0.25°	0.1x0.1°
model grids	360*180	720*360	1440*720	3600*1800
HPC cores	120	360	720	1800
HPC nodes	2	6	12	30
computing time	8 min/d	15 min/d	30 min/d	100 min/d
data volume	3 G/d	12 G/d	48 G/d	1 T/d

Spatial distribution of $PM_{2.5}$ concentration in Beijing and its surrounding areas

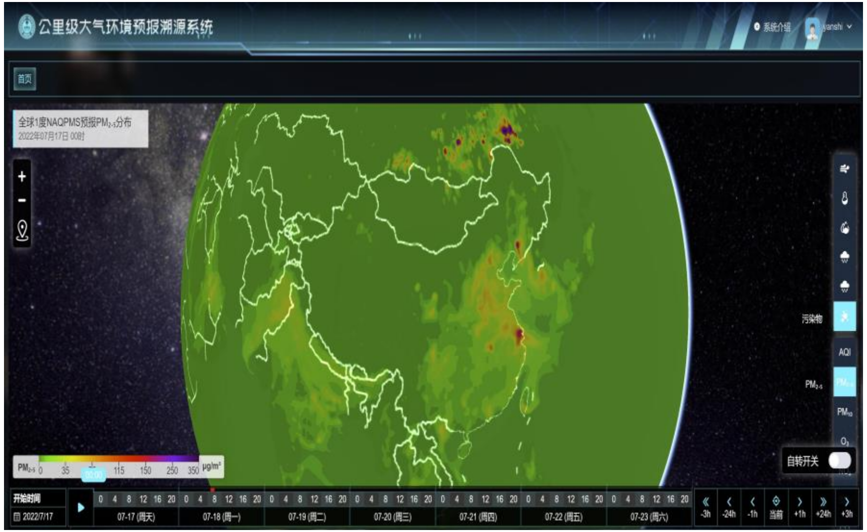


Application to global air quality forecasting

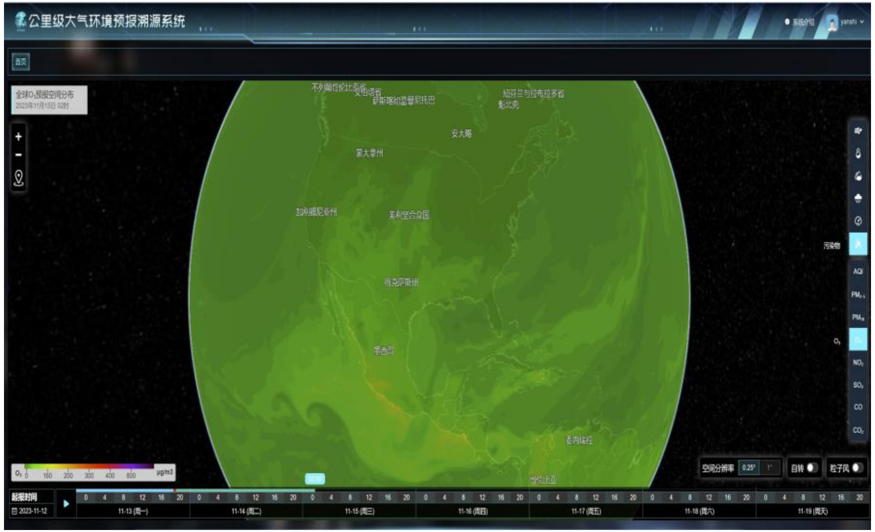
Two global forecasting systems with different resolutions have been constructed.

① 1.0x1.0° for 15-day forecasting, ② 0.25x0.25° for 7-day forecasting

$PM_{2.5}$ forecasting in East Asia



O_3 forecasting in North America



Emission inversion, model optimization and application

Advancing the representation of processes is not enough for application

Multi-source observation data

Advanced model

Data assimilation, emission inversion

Calculation optimization

Predict air quality, evaluate pollution effects, emission control, better air quality

Thanks for your attention

Thanks to all contributors & NSFC

Clean Air in Asia for Better Air Quality

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