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

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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**: ~200 µg m\(^{-3}\)
- **Clean Day**: ~25 µg m\(^{-3}\)

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

NAQPMS/GNAQPMS

- WRF
- IAP-AGCM

Tools
- KPP dealing with Chemical Equations
- Source Tagging
- Process Analysis
- Isotope Tracer

3-D Advection with global/regional option
- Chemical Reactions
  - Multi-phase Chemistry
  - Stratospheric Chemistry

- Turbulent Diffusion
- Dry Deposition
- Wet Scavenging

Aerosol Microphysics
- Multicomponent Nucleation
- Kinetic Condensation of SOA

Anthropogenic emissions

Online Emission of DMS, BVOC, NOx, NH₃, CO₂, CH₄, N₂O

IAP-DGVM

CNMM-DNDC

- Land
- Ocean
- Vegetation
- Soil

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
- Long-term simulation

Medium scheme
- Short-term coupled simulation

Detailed scheme
- 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

<table>
<thead>
<tr>
<th>mechanism</th>
<th>version</th>
<th>type</th>
<th>Inorganic reaction number</th>
</tr>
</thead>
<tbody>
<tr>
<td>RADM</td>
<td>RADM2</td>
<td>condensed</td>
<td>38</td>
</tr>
<tr>
<td>Carbon Bond</td>
<td>CB05</td>
<td>condensed</td>
<td>54</td>
</tr>
<tr>
<td>MOZART</td>
<td>MOZART-4</td>
<td>condensed</td>
<td>46</td>
</tr>
<tr>
<td>SAPRC</td>
<td>SAPRC07</td>
<td>condensed</td>
<td>55</td>
</tr>
<tr>
<td>RACM</td>
<td>RACM2</td>
<td>condensed</td>
<td>46</td>
</tr>
<tr>
<td>MCM</td>
<td>MCM3.3.1</td>
<td>near-explicit</td>
<td>45</td>
</tr>
<tr>
<td>MAX1</td>
<td>MAX1</td>
<td>condensed</td>
<td>60</td>
</tr>
</tbody>
</table>

MAX1 has good performance

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7
Develop tropospheric chemistry using KPP in GNAQPMS

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

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**GNAQPMS-stra model**

- **2 hpa**
- **Stratosphere 30layer**
- **100 hpa**
- **Troposphere 20layer**

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

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**Tropospheric chemistry** ($NO_x$-$VOC$-$CO$)

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Zhang et al., ERL, 2023
GNAQPMS has good skills in simulating stratospheric O₃

✓ Model reproduced observed ozone profiles in the stratosphere

Zonal and vertical distributions of stratospheric ozone

Comparison with WOUDC ozonesonde observations

GNAQPMS simulations

MLS Satellite

Zhang et al., 2023
Incorporating two schemes for photolysis rate calculation

TUV for troposphere simulation

O3MAP (Preprocess)
Satellite O3 column data

Tuv Table
(Clear sky photolysis)

ADJUST (online calculation)
Calculate aerosol and cloud effects

Fast-JX for troposphere & stratosphere

INPHOT (Prepare input)

Aerosols and cloud
Online simulated O$_3$ in troposphere & stratosphere

PHOTOJ

SOLARZ → SPHERE → EXTRA → OPMIE

OPTICL → OPTICA → OPTICM → JRATE
Consider HONO source and heterogeneous mechanism

Add new emission sources and heterogeneous reaction pathways

- Soil emission, indoor emission, biomass burning and updated mobile emission
  \[ F_N(\text{HONO}) = F_{N,\text{opt}}(\text{HONO}) \times e^{\frac{E_d}{R_\text{opt}T_\text{opt}}} \times f(\text{SWC}) \]

- New heterogeneous reactions
  1. \([200:H29] \text{NO}_2 + \text{SGRND} = \text{HONO}\)
  2. \([201:H30] \text{NO}_2 + \text{PAER} = 0.5 \text{HONO}\)
  3. \([202:H31] \text{AERNO}_3 + \text{SGRND} + \text{hv} = 0.67 \text{HONO} + 0.33 \text{NO}_2\)
  4. \([203:H32] \text{HNO}_3 + \text{SGRND} + \text{hv} = 0.67 \text{HONO} + 0.33 \text{NO}_2\)
  5. \([204:H33] \text{AERNO}_3 + \text{hv} = 0.67 \text{HONO} + 0.33 \text{NO}_2\)

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

The overestimation at nighttime and the underestimation of HONO at daytime were significantly improved
The Mn-catalytic heterogeneous reactions increase sulfate chemical production and remarkably reduce model biases.

**Sulfate formation scheme in WRF-Chem**

- **Gas phase**
  \[ \text{SO}_2 + \text{OH} + \text{H}_2\text{O} + \text{O}_2 \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2 \]

- **Aqueous phase**
  \[ \text{HSO}_3^- + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + \text{H}^+ + \text{H}_2\text{O} \]
  \[ \text{SO}_2 + \text{O}_3 + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + 2\text{H}^+ + \text{O}_2 \]
  \[ \text{SO}_2 + \text{H}_2\text{O} + 0.5\text{O}_2 + \text{Fe}^{3+}/\text{Mn}^{2+} \rightarrow \text{SO}_4^{2-} + 2\text{H}^+ \]
  \[ \text{HSO}_3^- + 2\text{NO}_2 + \text{H}_2\text{O} \rightarrow \text{SO}_4^{2-} + 3\text{H}^+ + 2\text{NO}_2^- \]

**New sulfate scheme by Wang et al. (2021)**

- **Transition metal-catalyzed oxidation of SO2 on aerosol surfaces**
  \[ \text{SO}_2 + \text{O}_2 + \text{Mn(OH)}_{x/3} \rightarrow \text{SO}_5^- + \text{Mn}^{2+}, \ x = 1, 2 \]
  \[ \text{SO}_5^- + \text{Mn}^{2+} + \text{H}^+ \rightarrow \text{Mn(OH)}_{x/3} + \text{HSO}_5^- \]
  \[ \text{NH}_3 + \text{HSO}_5^- + \text{SO}_2 + \text{H}_2\text{O} \rightarrow \text{NH}_4^+ + \text{SO}_4^{2-} \]
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)

Model reproduced SOA and SOA/OA

Systematic underestimation!
(Kanakidou&Swietlicki, 2005; Lin et al., 2016)
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 (12D-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**
Online calculation of natural trace gases in GNAQPMS

Online emission of **DMS**
depending on seawater DMS concentration, wind, and sea surface temperature

![DMS concentration in seawater](image1)

![DMS emission](image2)

Wei et al., ACP, 2019

Online emission of **BVOCs**
depending on vegetation and meteological factors

![Isoprene emission at 00:00](image3)

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 processes

Nucleation rates

Reproduced the New Particle Formation events

Chen et al., ACP, 2021
Parameterized minimum eddy diffusivity ($K_{z\text{min}}$) for improving PM$_{2.5}$ simulations under stable Boundary Layer

$$K_h = kw_s z \left(1 - \frac{z}{h}\right)^2 / Pr + K_{z\text{min}}$$

$$K_{z\text{min}} = 1 + LE/H$$

**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

\[ x^a = x^b + BH^T(HBH^T + R)^{-1}(y^o - Hx^b) \]

Background error  Observation error

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

\[ -2L(\lambda) = \ln\{\det(H\lambda P_e H^T + R)\} + d^T H\lambda P_e H^T + R)^{-1} d \]

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

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)
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

<table>
<thead>
<tr>
<th></th>
<th>NOx</th>
<th>SO2</th>
<th>CO</th>
<th>PM2.5</th>
<th>PM10</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1 (Gg/day)</td>
<td>72.9</td>
<td>23.8</td>
<td>1160.2</td>
<td>44.5</td>
<td>75.5</td>
</tr>
<tr>
<td>P2 (Gg/day)</td>
<td>41.9</td>
<td>21.5</td>
<td>1037.4</td>
<td>40.9</td>
<td>66.4</td>
</tr>
<tr>
<td>P3 (Gg/day)</td>
<td>44.8</td>
<td>23.2</td>
<td>1078.2</td>
<td>45.9</td>
<td>108.4</td>
</tr>
</tbody>
</table>

\[
\frac{(P2 - P1)}{P1} \quad -42.5\% \quad -9.7\% \quad -10.6\% \quad -7.9\% \quad -12.1\%
\]

\[
\frac{(P3 - P1)}{P1} \quad -38.6\% \quad -2.5\% \quad -7.0\% \quad 3.3\% \quad 43.6\%
\]
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-emission > 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.
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.

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

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

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
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**

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

**Spatial distribution of PM$_{2.5}$ concentration in Beijing and its surrounding areas**

- 1°x1°
- 0.5°x0.5°
- 0.25°x0.25°
- 0.1°x0.1°
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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