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Application of Korean Air Quality Modeling System named GMAF to Winter and Spring in 2018

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CONTENTS

1. Introduction

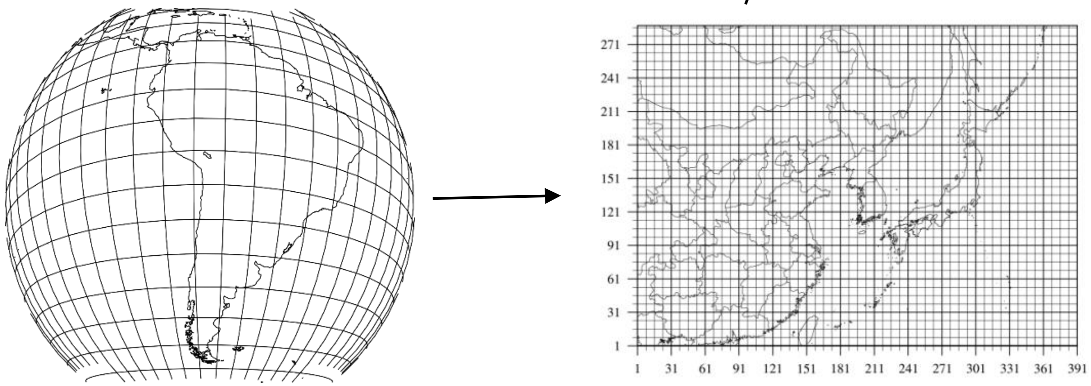
Description of GMAF

- Operate global and mesoscale model system separately.

- Global forecasting data was linked to regional scale modeling by **grid nudging based on FDDA** instead of surface monitoring data .

GMAF

Global to **M**esoscale **A**ir quality **F**orecasts and analysis



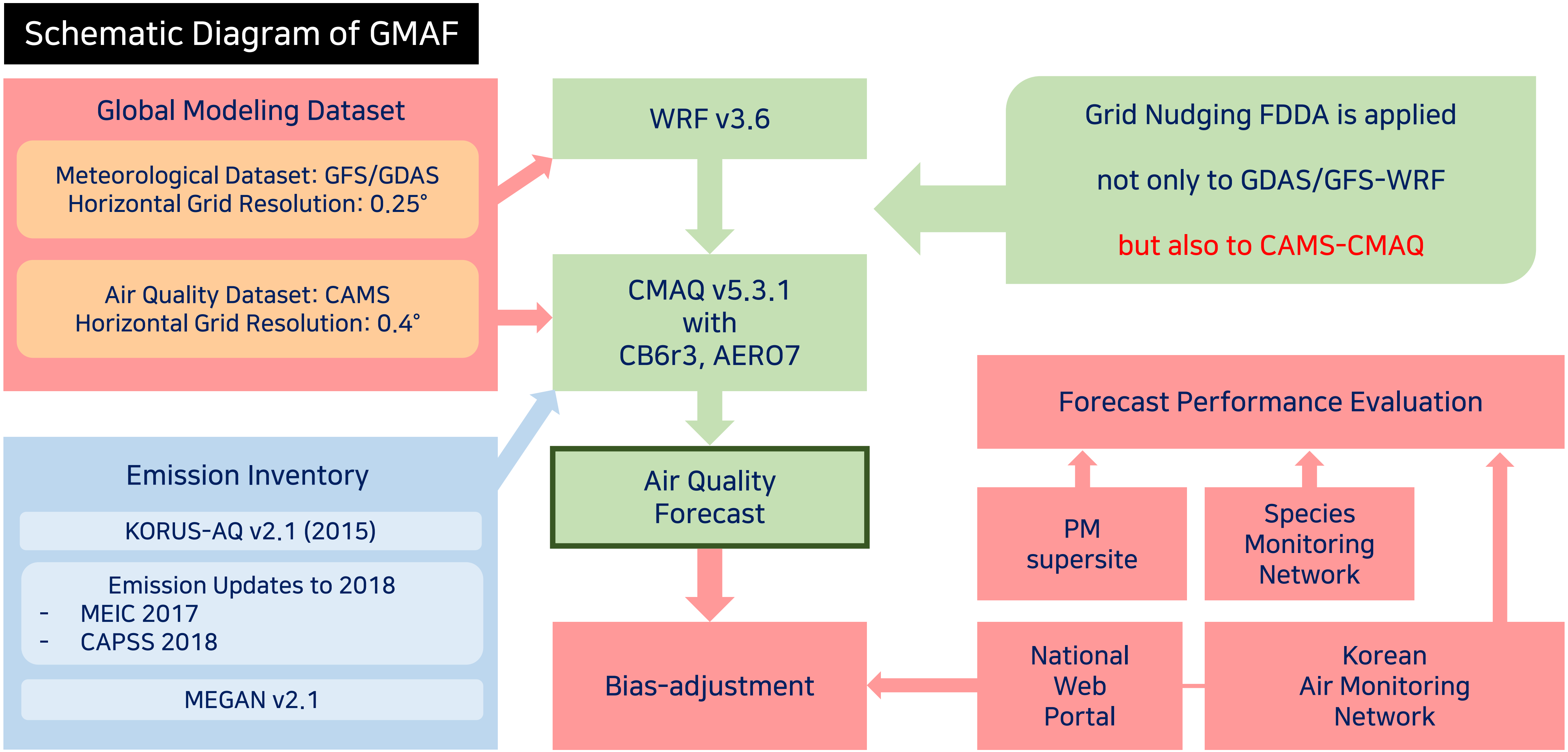
CAMS CMAQ

Global to Mesoscale Air Quality Forecast and analysis (GMAF) system

was developed by Cho et al. (2021)

and used for application to Korean air quality from January 2018 to March 2018.

1. Introduction



2. Modification of CMAQ

Below-cloud Scavenging

* CMAQ assumes absorption of all accumulation and coarse mode particles in the droplets.

$$\Lambda_c = 4.2 \times 10^{-7} \frac{E(d_p)P}{d_d}$$: wet scavenging coefficient

$$E(d_p) = \frac{4}{R_e S_c}\left(1 + 0.4R_e^{\frac{1}{2}}S_c^{\frac{1}{3}} + 0.16R_e^{\frac{1}{2}}S_c^{\frac{1}{2}}\right) + 4\emptyset\left[\frac{\mu}{\mu_w} + \emptyset\left(1 + 2R_e^{\frac{1}{2}}\right)\right] + \left(\frac{S_t - S^*}{S_t - S^* + 2/3}\right)^{3/2}$$: Raindrop-Aerosol collision Efficiency

* R_e: Reynolds number, S_c: Schmidt number, S_t: Stokes number

$$d_d = 9 \times 10^{-4} P^{0.21}$$: diameter of droplet (mm/hr)

$$P = \frac{10^7 L_p}{\rho_w}^{1.27}$$: rainfall rate (mm/hr)

Modification of below-cloud scavenging mechanism improved the model performance by resolving underestimation of particles.

2. Modification of CMAQ

Vertical Mixing

Vertical eddy diffusivity calculation

CMAQ ver 4: $K_{z,min} = K_{ZL} + (K_{ZU} - K_{ZL}) * F_{urban}$ $K_{ZL} = 0.5$ $K_{ZU} = 2.0$

CMAQ ver 5: $K_{z,min} = K_{ZL} + (K_{ZU} - K_{ZL}) * F_{urban}$ $K_{ZL} = 0.01$ $K_{ZU} = 1.0$

→ $K_{z,min}$ of CMAQ v5.3.1 is too low and leads to suppression of diffusion in the stable atmosphere (mainly night).

→ Subsequently, it causes overestimation of air pollutants concentration at the surface.

2. Modification of CMAQ

N_2O_5 uptake coefficient

- Overestimation of particulate nitrate by CMAQ's default version of N_2O_5 uptake coefficient (Davis et al., 2008).
- Applying **organic coating inhibition on the aerosol** based on Anttila et al. (2006) to resolve overestimation of nitrate.

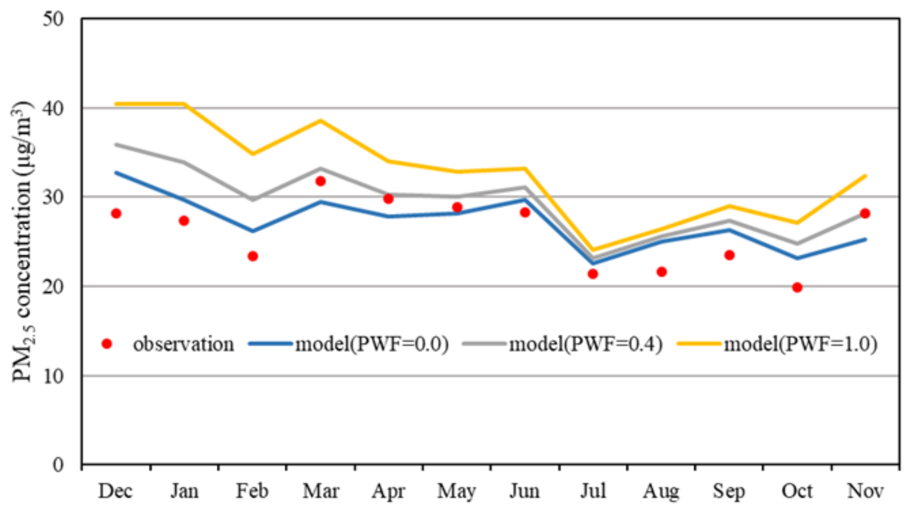
$$\frac{1}{\gamma_{N2O5}} = \frac{1}{\gamma_{N2O5,core}} + \frac{1}{\gamma_{N2O5,coat}}$$

$\gamma_{N2O5,core}$: formula of Davis et al. (2008)

$\gamma_{N2O5,coat}$: organic coating inhibition (=0.0012)

Parameter of pcVOC

- pcVOC emission = factor * POA emission
- Overestimation of OA concentration due to high pcSOA concentration.
- Lowering pcVOC emission scale factor from 6.579 to 2.6316 based on sensitivity run by Cho et al. (2021).



3. Grid Nudging

CAMS global atmospheric composition forecast data

IFS
(Integrated
Forecasting System)
by ECMWF

4D-VAR
Data assimilation

Polar orbiting
Satellite Data

- **Frequency:** twice a day (00:00 and 12:00 UTC)

- **Forecast hours:** 120 hours forecasts with 3 hours interval

- **Resolution:** 40km (horizontal), 137 levels (vertical)

- **Gaseous species:** SO_2, HCHO, NO, NO_2, O_3, PAN, CH_4, Isoprene, OH, HNO_3 etc. 56 reactive traces gases in the troposphere and stratospheric O_3

- **Aerosol species:** Dust, Sea-salt, organic matter, black carbon, sulfate, nitrate, ammonium

3. Grid Nudging

Grid Nudging based on FDDA

The grid nudging based on FDDA adds a relaxation term that is supposed to force the observations to the model as Eq. (1).

$$\frac{dY_{model}}{dt} = F(x, Y_{model}) + W(x)(Y_{obs} - Y_{model}) \quad (Eq. 1)$$

Y: dependent variable

F: discretized form of the governing equation

x: independent spatial variable

W: nudging coefficient

$$Y = \alpha\left(P_{top} - P_{surface}\right) \quad \text{for the WRF} \quad (Eq. 2)$$

$$Y = \varphi J_s \quad \text{for the CMAQ} \quad (Eq. 3)$$

α: meteorological variable of the WRF

φ: chemical species mass concentration

P_{top}: air pressure at the top of the domain

$P_{surface}$: air pressure at the surface

J_s: vertical Jacobian of the terrain-influenced coordinates

3. Grid Nudging

Grid Nudging based on FDDA

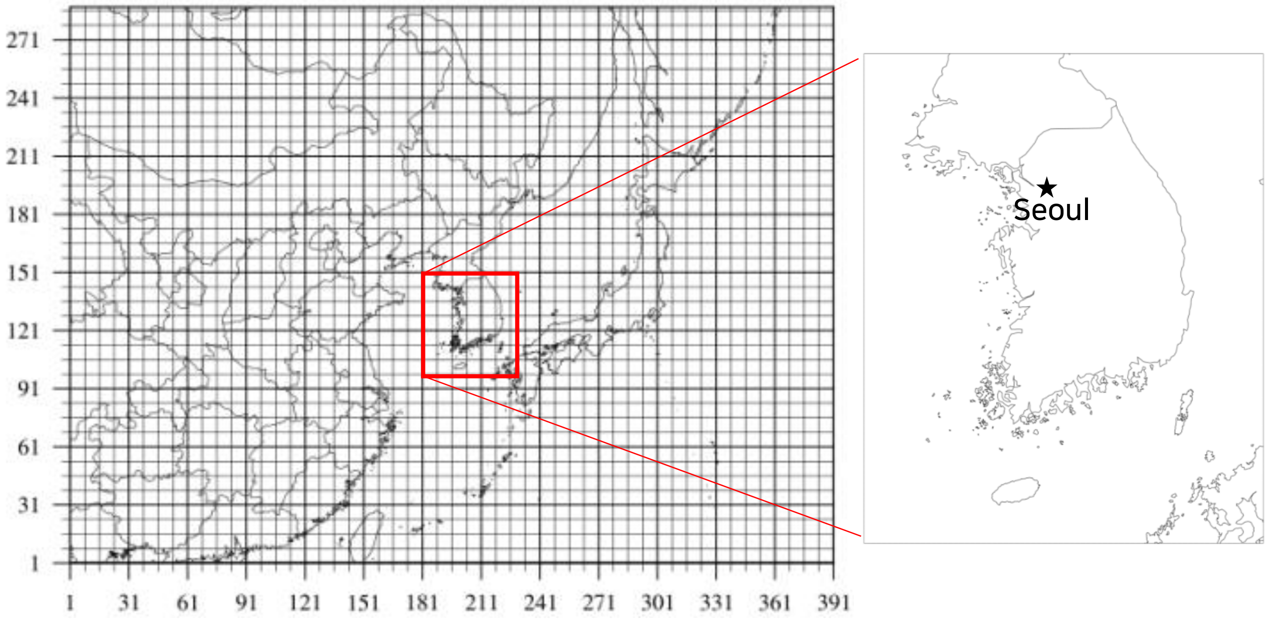
	Nudged Variable	Nudging Coefficient	
		Outer Domain	Inner Domain
WRF	U and V winds	5.0×10^{-4}	2.5×10^{-4}
	Temperature	5.0×10^{-4}	2.5×10^{-4}
	Water vapor mixing ratio	1.0×10^{-4}	1.0×10^{-4}
CMAQ	SO_2, NO, NO_2, O_3, dust, sea-salt, isoprene, CO	3.0×10^{-4}	0

- The nested domain used nudging coefficient as same as the table.

- The uniform domain used nudging coefficient as same as ‘outer domain’, and the grid nudging based on FDDA were not applied to South Korea.

4. Model Results

Model Configuration



Model domain

- 391 columns X 288 rows
- 12 km grid spacing (uniform grid)

Period: January 2018 to March 2018

Model structure

- Chemical transport model: CMAQ version 5.3.1
- Meteorological model: WRF version 3.6
- Emissions: MEIC 2017, CAPSS 2018, KORUS v2.1, MEGAN version 2.1
- Aerosol dynamics: AERO7
- Gas-phase chemistry: 3rd release of carbon bond 6

4. Model Results

$PM_{2.5}$ prediction

$$R = \frac{\sum_{i=1}^{i=N}(O_i - \bar{O})(M_i - \bar{M})}{\sqrt{\sum_{i=1}^{i=N}(O_i - \bar{O})^2}\sqrt{\sum_{i=1}^{i=N}(M_i - \bar{M})^2}}$$

Goal > 0.70
Criteria > 0.40

$$\text{NMB (\%)} = \frac{\bar{M} - \bar{O}}{\bar{O}} \times 100$$

Goal $< \pm 10\%$
Criteria $< \pm 30\%$

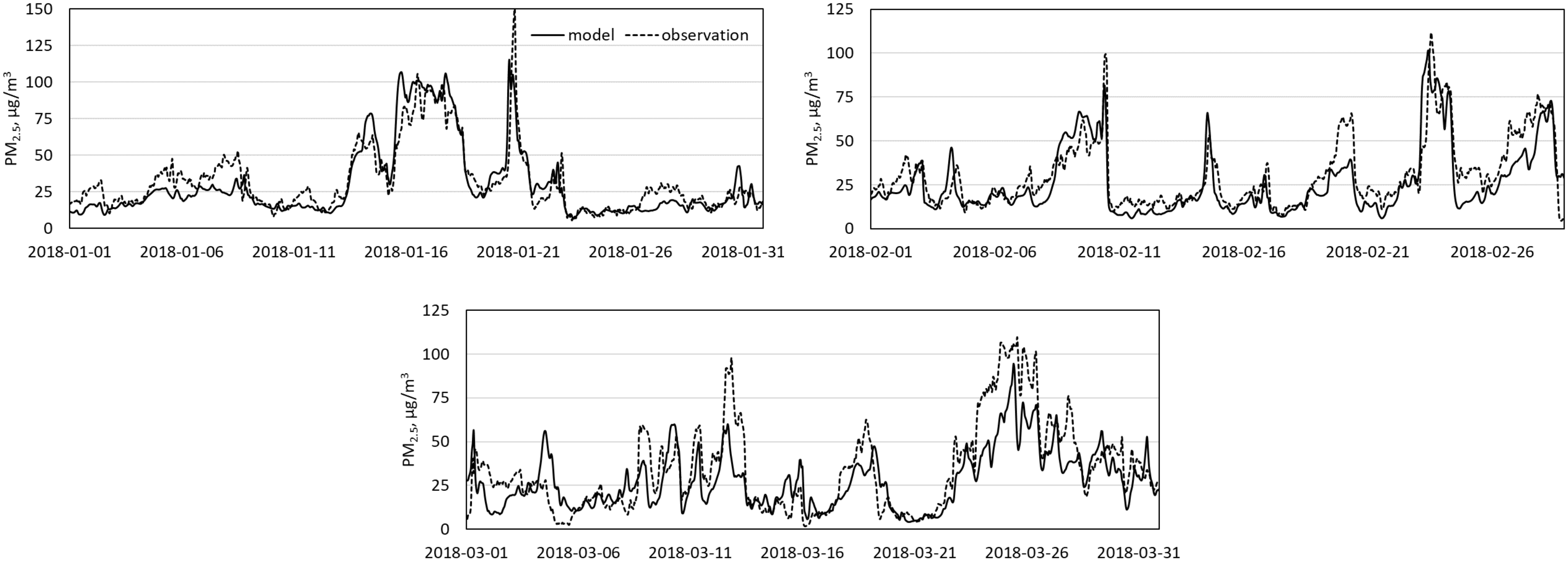
$$\text{NME (\%)} = \frac{\frac{1}{N}\sum_{i=1}^{i=N}|M_i - O_i|}{\bar{O}} \times 100$$

Goal $< \pm 35\%$
Criteria $< \pm 50\%$

	Avg. Observation (μg/m³)	Avg. Model (μg/m³)	R	NMB (%)	NME (%)
Jan, 2018	32.23	32.10	**0.96**	**-0.1**	20
Feb, 2018	30.24	27.53	0.90	-9	20
Mar, 2018	34.13	30.13	0.88	-12	28
Total	32.27	30.00	**0.88**	**-7**	23

4. Model Results

$PM_{2.5}$ prediction



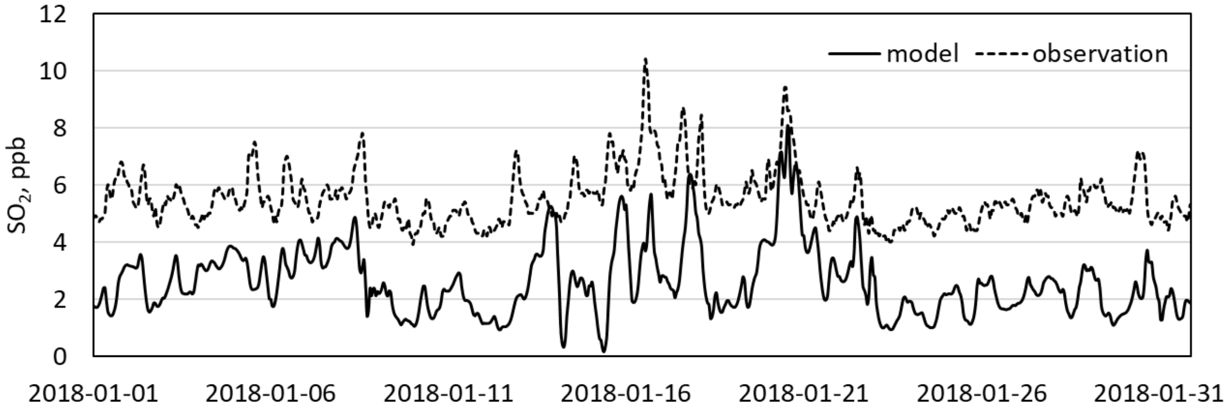
4. Model Results

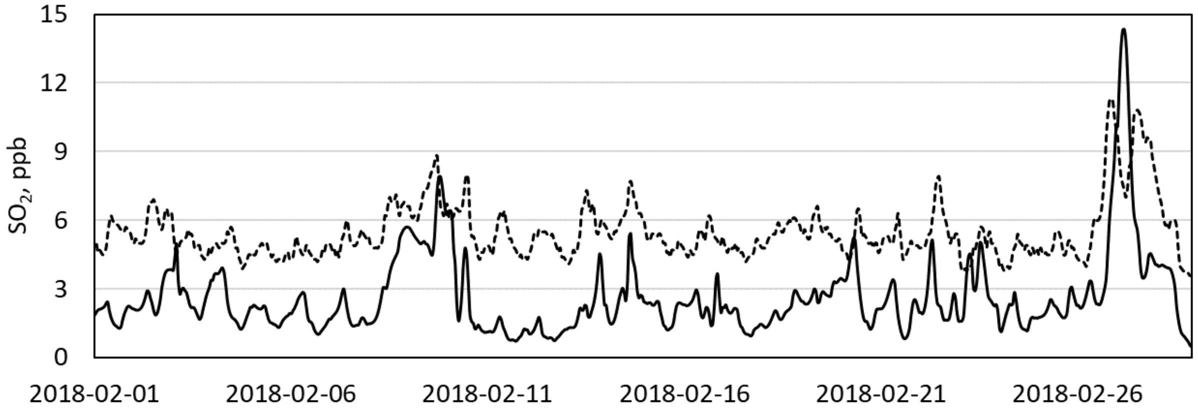
SO_2 prediction

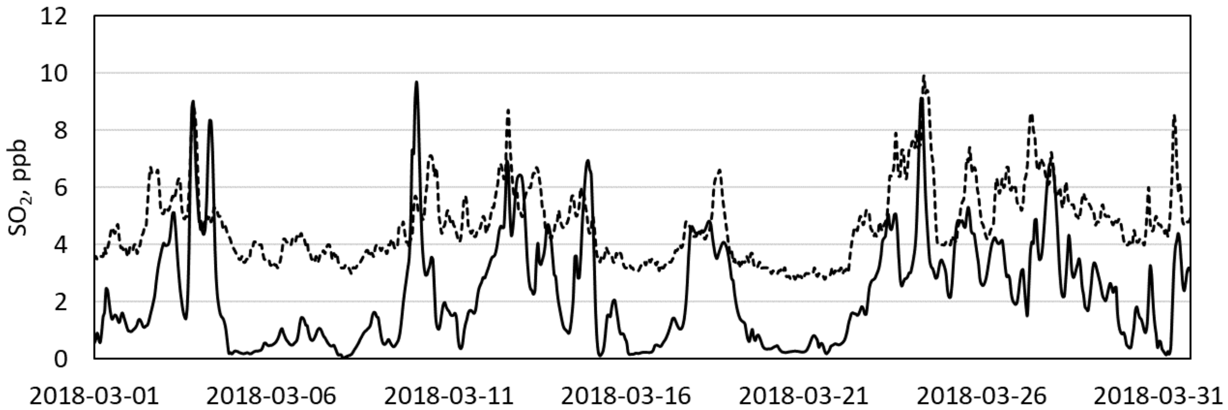
	Avg. Obs	Avg. model	R	NMB (%)	NME (%)
Jan, 2018	5.5	2.6	0.56	-53	53
Feb, 2018	5.5	2.6	0.61	-52	54
Mar, 2018	4.7	2.3	0.69	-51	54
Total	5.2	2.5	0.63	-52	54

4. Model Results

SO_2 prediction







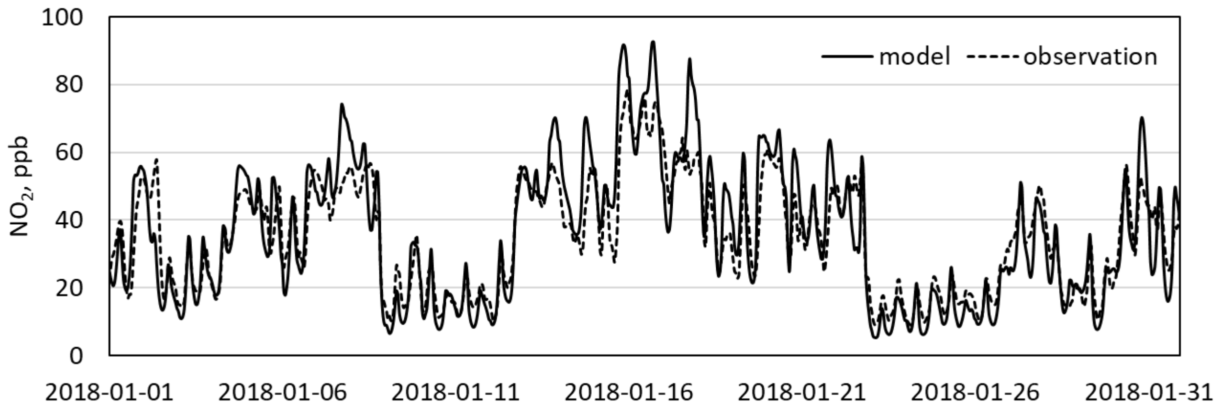
4. Model Results

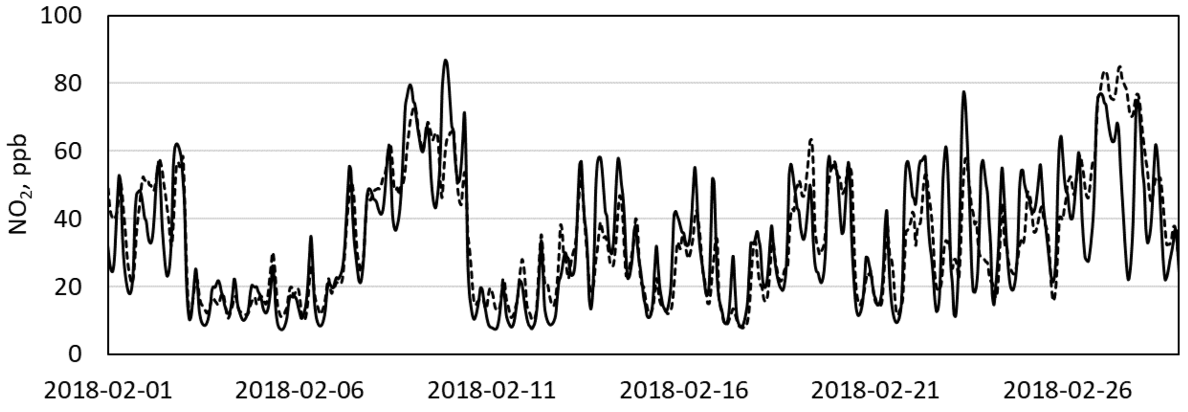
NO_2 prediction

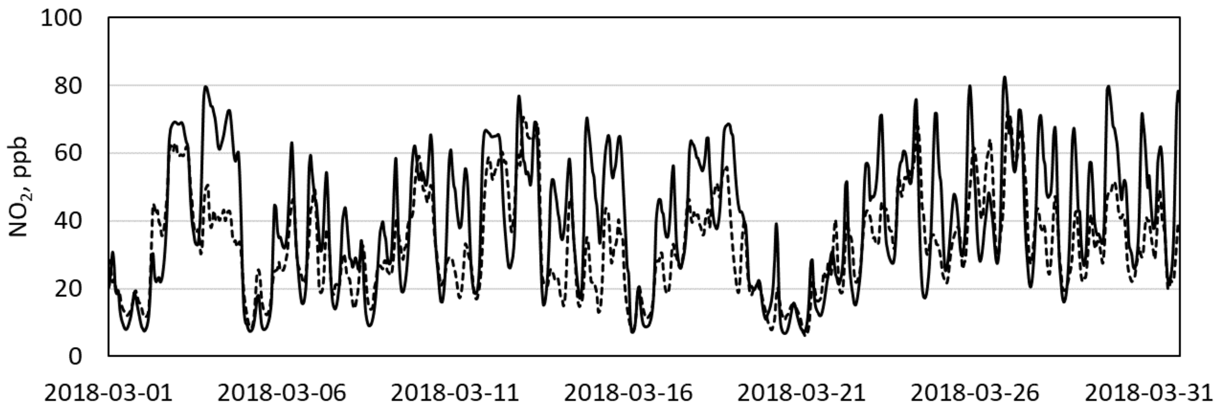
	Avg. Obs	Avg. model	R	NMB (%)	NME (%)
Jan, 2018	35.0	35.8	0.91	2.3	17.6
Feb, 2018	34.1	33.3	0.83	-2.2	22.1
Mar, 2018	33.1	39.9	0.75	20.3	33.7
Total	34.1	36.4	0.82	6.9	24.4

4. Model Results

NO$_2$ prediction







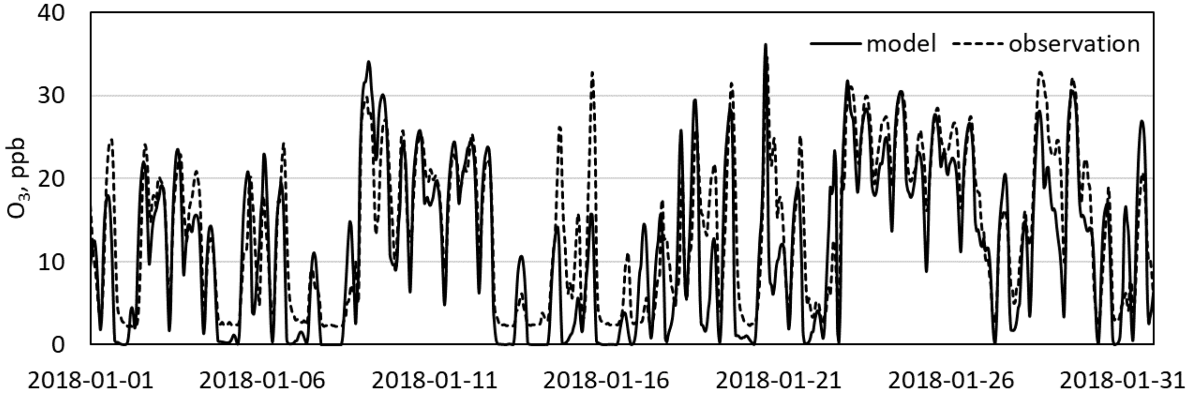
4. Model Results

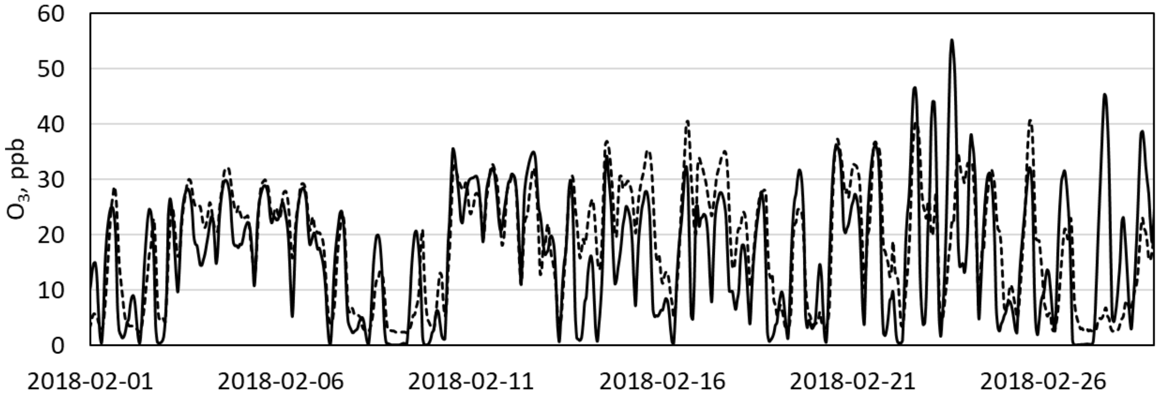
O_3 prediction

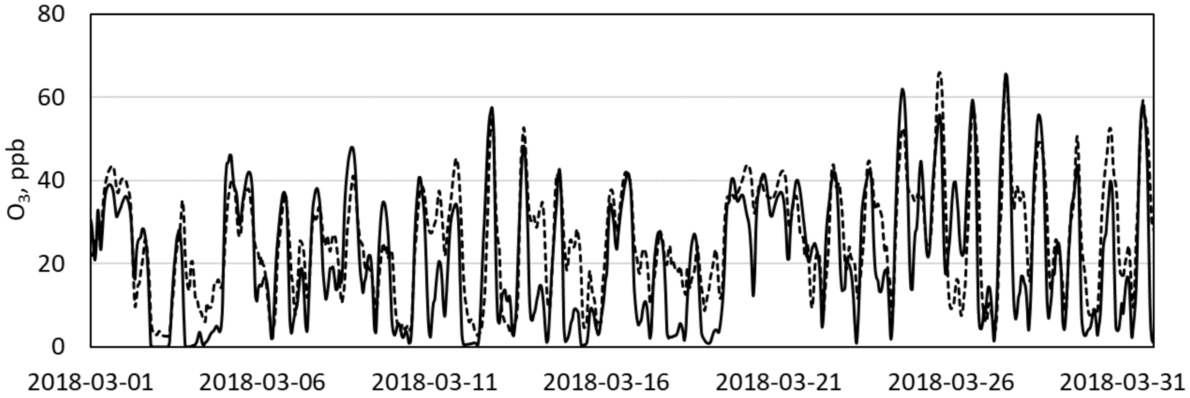
	Avg. Obs	Avg. model	R	NMB (%)	NME (%)
Jan, 2018	13.7	11.9	0.85	-13.2	28.9
Feb, 2018	18.3	16.8	0.70	-8.1	33.9
Mar, 2018	25.8	21.5	0.79	-16.8	31.4
Total	19.3	16.7	0.80	-13.4	31.5

4. Model Results

O_3 prediction







5. Summary

- We conducted a model simulation using the WRF-CMAQ framework named GMAF from January to March 2018.

- The GMAF applied grid nudging based on FDDA not only to the WRF but also to CMAQ.

- The vertical eddy diffusivity, below-cloud wet scavenging, calculation of N_2O_5 uptake coefficient, and parameter of pcVOC in CMAQ were modified.

- The model performance for predicting $PM_{2.5}$, SO_2, NO_2, and O_3 was evaluated by R, NMB, and NME.

- The model results showed reasonably good agreement with observation in prediction of $PM_{2.5}$, NO_2, and O_3.

Reference

Cho et al. (2021) Development of the Global to Mesoscale Air Quality Forecast and Analysis System (GMAF) and Its Application to $PM_{2.5}$ Forecast in Korea, Atmosphere.

Davis et al. (2008) Parameterization of N_2O_5 reaction probabilities on the surface of particles containing ammonium, sulfate, and nitrate, Atmospheric Chemistry and Physics.

Anttila et al. (2006) On the reactive uptake of gaseous compounds by organic-coated aqueous aerosols: Theoretical analysis and application to the heterogeneous hydrolysis of N_2O_5, The Journal of Physical Chemistry A.