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Weakly coupled data assimilation with aerosol-cloud interactions in WRF-Chem/WRFDA

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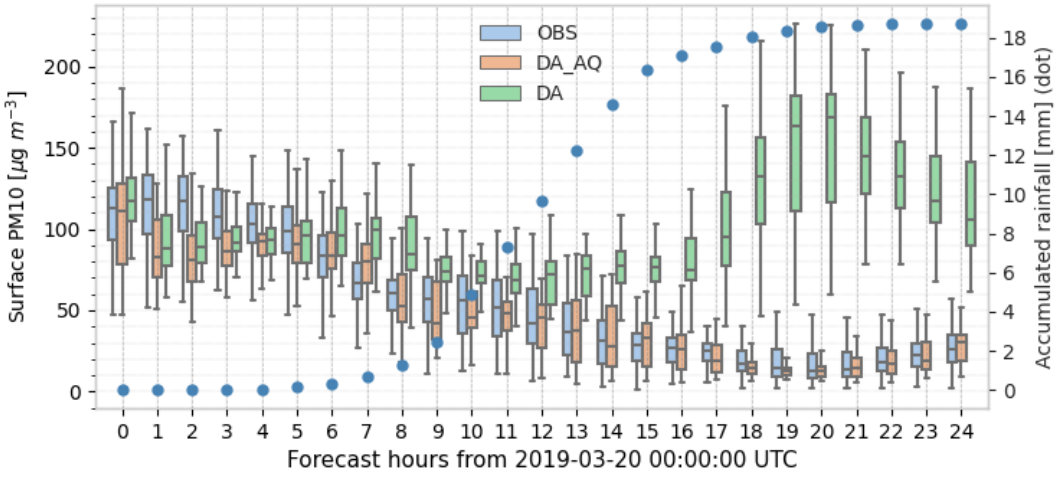


WRF/MPAS Users' Workshop on Jun 7, 2022

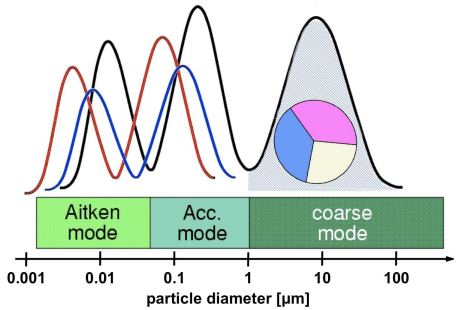
Background – Developments for aerosol DA in WRF-Chem/WRFDA

- To improve air-quality forecasting, new assimilation capabilities have been developed using the RACM/MADE-VBS chemistry scheme (Tuccella et al. 2015; WRF V3.4) in WRF-Chem/WRFDA for the last few years.

: chem_opt = 108 in WRF-Chem/WRFDA was released in WRF V4.4 (Ha, GMD2022).

⇒Gas-phase mechanism: Regional Atmospheric Chemistry Mechanism (RACM; Stockwell et al., 1997) in WRF-Chem.

⇒Inorganic aerosols: Modal Aerosol Dynamics Model for Europe (MADE; Ackermann et al., 1998), defining the aerosol particle size distribution as a superposition of three log-normal modes.
⇒Secondary Organic Aerosol (SOA) is produced based on the Volatility Basis Set (VBS) approach (Ahmadov et al., 2012).



Aquila et al. (GMD 2011)

- Weakly coupled DA:
  - Simultaneous but independent assimilation of MET and CHEM observations in WRFDA
  - MET and CHEM variables are fully coupled only in WRF-Chem forecasts.

Background – Expansion of WRF-Chem/WRFDA to aqueous chemistry

Eck et al. (2018): Major aerosol pollution transport events over East Asia were often associated with extensive cloud cover, changing aerosol size distribution, but hard to be observed.

=> Underrepresented in the remote-sensing data.

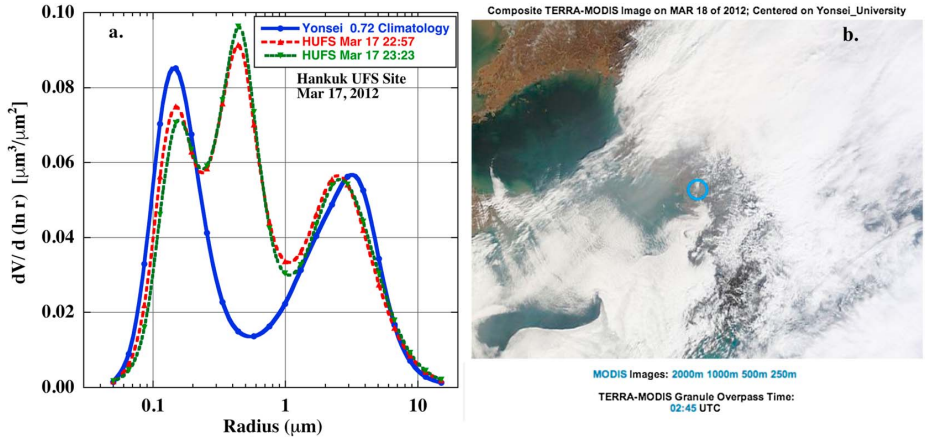
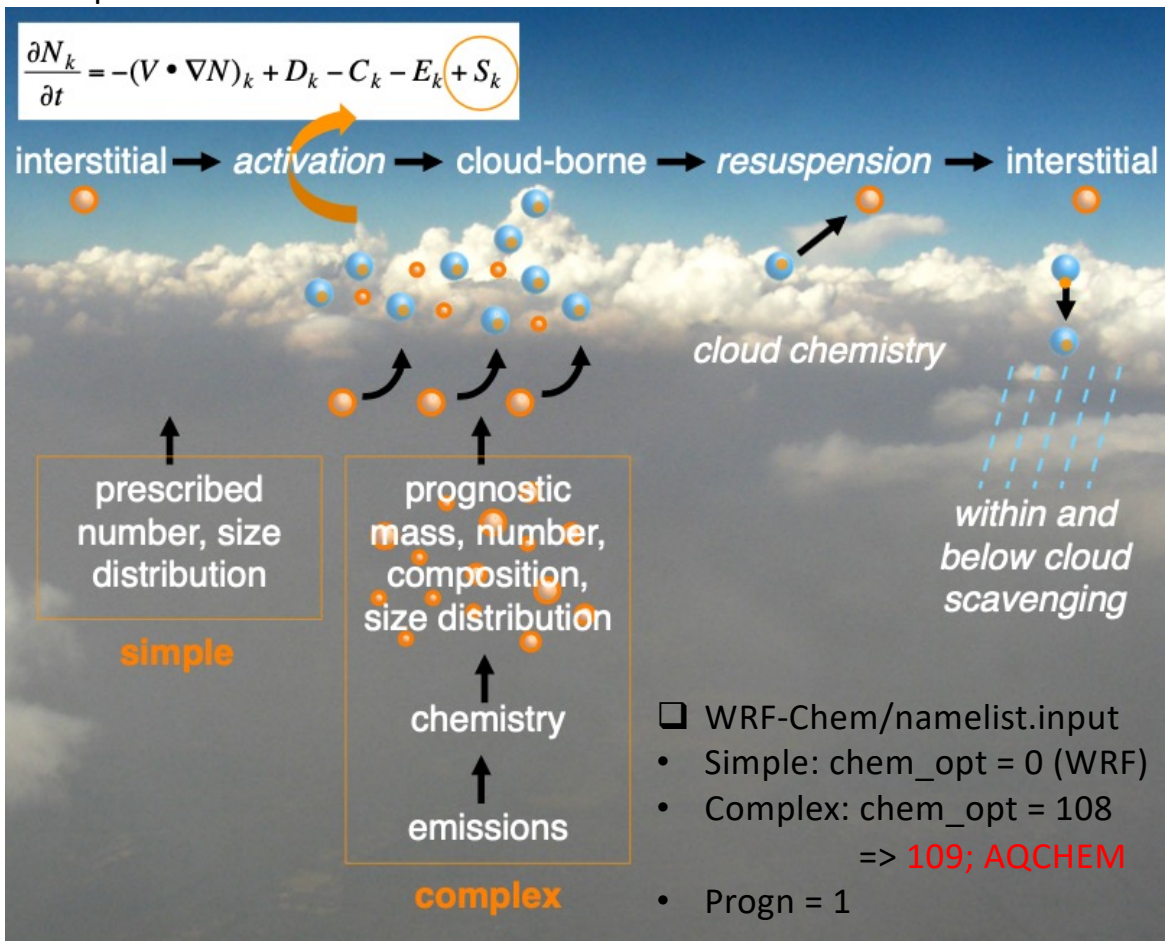


Figure 6. (a) Almucantar retrievals of aerosol size distributions from Aerosol Robotic Network measurements made at the Hankuk UFS site on 17 March 2012, as compared to climatological mean size distributions from the Yonsei University site utilizing 42 retrievals from March to May 2011 and 2012 with average fine mode fraction (440 nm) of 0.88 and AOD(440 nm) ranging from 0.6–0.8. (b) MODIS Terra image from about 4 hr after the Hankuk UFS retrievals shown in (a). The blue circle indicates the Yonsei University site location. MODIS = Moderate Resolution Imaging Spectroradiometer.

- The lack of observations makes it more critical to reduce model error (e.g., w/ advanced physics).
- Aqueous Chemistry (AQCHEM) is required to simulate aerosol-cloud interactions in WRF-Chem.

Aerosol-cloud interactions w/ aqueous chemistry in WRF-Chem

Adopted from WRF-Chem Tutorial 2013



To interact with clouds, aerosols in cloud water (cw) should exist. => "Aqueous chemistry"

- ❑ Aqueous Chemistry - coupled to Lin and Morrison double-moment microphysics.
- ❑ Wet removal: cloud-borne aerosols are collected by both grid-scale and convective precipitation (rain, snow, graupel).
- ❑ Without AQCHEM, aerosols cannot directly affect the formation/growth of clouds and cannot be displaced through convective transport or removed by wet scavenging.

Aerosol data assimilation in WRFDA 3DVAR

$$J(\mathbf{v}) = \frac{1}{2}\mathbf{v}^{\mathbf{T}}\mathbf{v} + \frac{1}{2}(\mathbf{d} - \mathbf{H}\mathbf{B}^{1/2}\mathbf{v})^{\mathbf{T}}\mathbf{R}^{-1}(\mathbf{d} - \mathbf{H}\mathbf{B}^{1/2}\mathbf{v}) \quad \text{where} \quad \mathbf{d} = \mathbf{y} - \mathbf{H}(\mathbf{x_b}) \text{ and } \mathbf{B}^{1/2} = \mathbf{U_p}\mathbf{S}\mathbf{U_v}\mathbf{U_h}$$

Control variables (**v**), Background error covariance (**B**), Observation operator **H(x)**, observations (**y**) are all composed of MET fields + gas and aerosol fields defined in RACM/MADE-VBS.

For $PM_{2.5}$ assimilation,

$$\mathbf{H(x)}: PM_{2.5} = \rho_d \sum_{k=i}^{j}[SO_4^k + NO_3^k + NH_4^k + Cl^k + POM^k + EC^k + Na^k + P25^k + \sum_{m=1}^{4}[ASOA_m^k + BSOA_m^k]]$$

$$\mathbf{H(x)}: PM_{2.5} = \rho_d \sum_{k=i}^{j}[SO_4^k + NO_3^k + NH_4^k + Cl^k + POM^k + EC^k + Na^k + P25^k + \sum_{m=1}^{4}[ASOA_m^k + BSOA_m^k]]$$
$$+ \rho_d \sum_{k=cwi}^{cwj}[SO_4^k + NO_3^k + NH_4^k + Cl^k + POM^k + EC^k + Na^k + P25^k + \sum_{m=1}^{4}[ASOA_m^k + BSOA_m^k]]$$

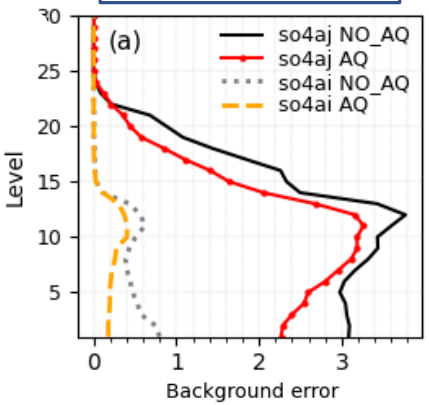
i: Aitken
j: Accumulation mode

- Interstitial and cloud-borne aerosol particles are treated explicitly.
- For each aerosol species, cloud-borne particles (cw) in three different modes are added in control variables (v), observation operator ($H(x)$), its tangent linear(H) and adjoint (H^T) versions, and background error covariance (B).

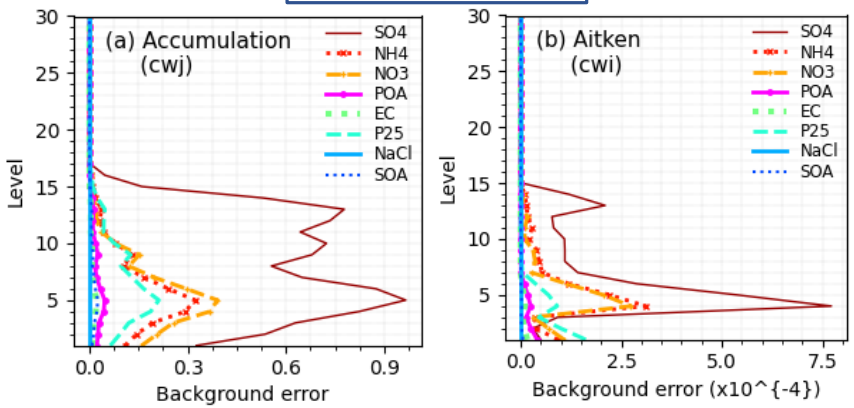
Background error covariance with aerosol species (**B**)

- **B** is critical in spreading out the observed information (H/V) and to weigh aerosol species in the assimilation of surface PM concentration.
- cv_options = 7: All control variables (u, v, t, rh, w, ps) are full fields;
  No cross-correlations for chem variables.
- GENBE 2.0 is expanded for chem_opt=109, increasing total no. of variables from 45 to 80 (= 74 chem + 6 met).
- Aqueous Chemistry (AQ) mostly affects the oxidation of S(IV) in the mid-to-low troposphere, reducing sulfate in the interstitial phase while significantly increasing cloud-borne sulfate in the accumulation mode (cwj).

Interstitial phase

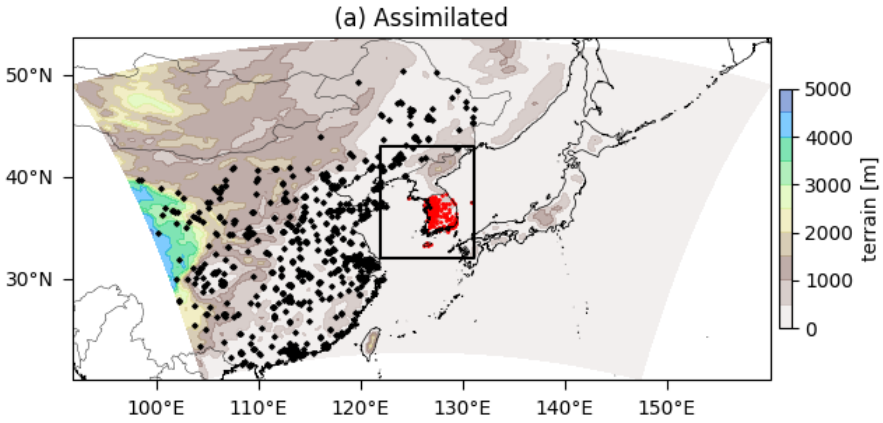


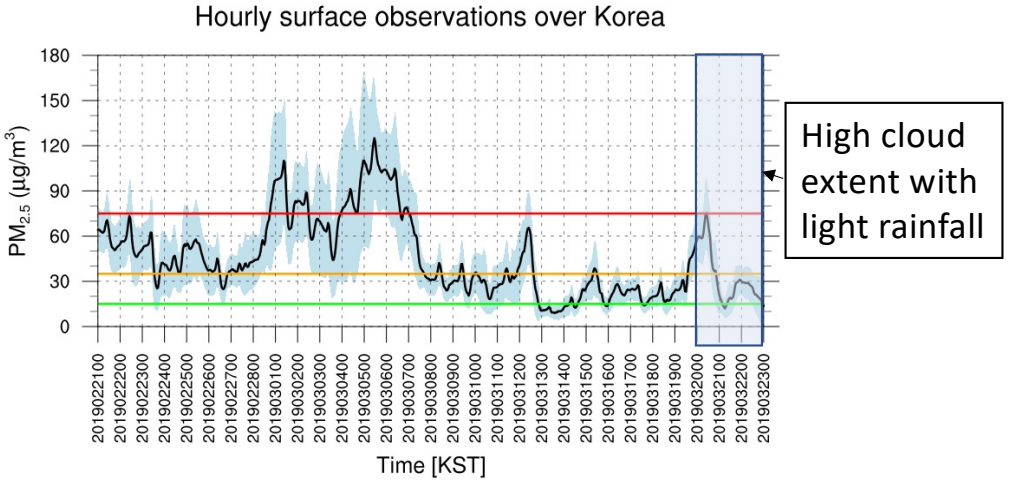
Aqueous phase



Cycling experiments

- One-way nesting in 27- and 9-km grids; 31 vertical levels up to 50 hPa
- Assimilate surface PM_{10} and $PM_{2.5}$ observations every 6 h for Feb 21-Mar 21, 2019.
- chem_opt = 108 => 109 (racm_soa_vbs_aqchem_kpp)
- Morrison/RRTMG/Grell-3/YSU/Noah physics with aerosol direct and indirect effects

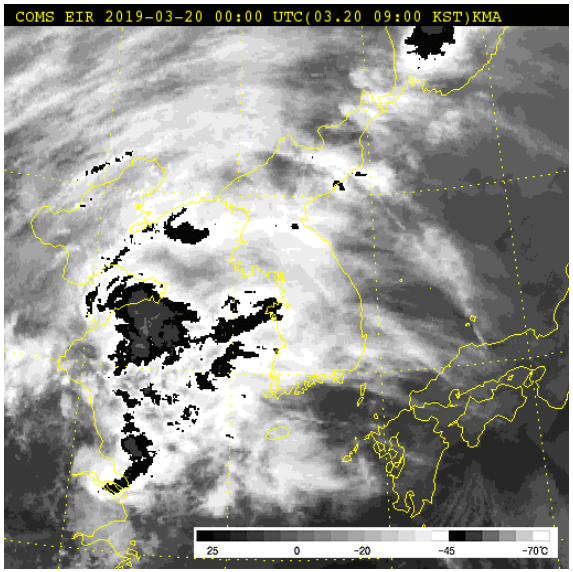




Concentration	Good	Moderate	Unhealthy	Very Unhealthy
$PM_{2.5}$ [$\mu g/m^3$]	15	35	75	> 75
PM_{10} [$\mu g/m^3$]	30	80	150	> 150

Aerosol data assimilation with AQCHEM

- A pollution event w/ high cloud cover on 20 March 2019.



Experiment	chem_opt	Assimilation
NODA	108	None
DA	108	CHEM+MET
NODA_AQ	109	None
DA_AQ	109	CHEM+MET

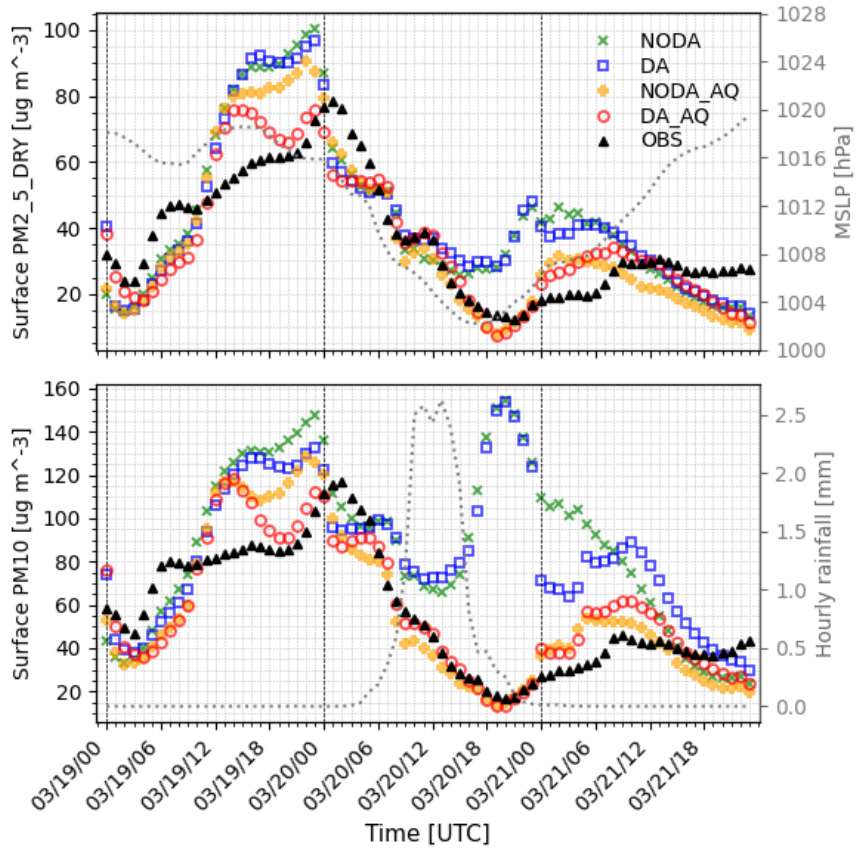
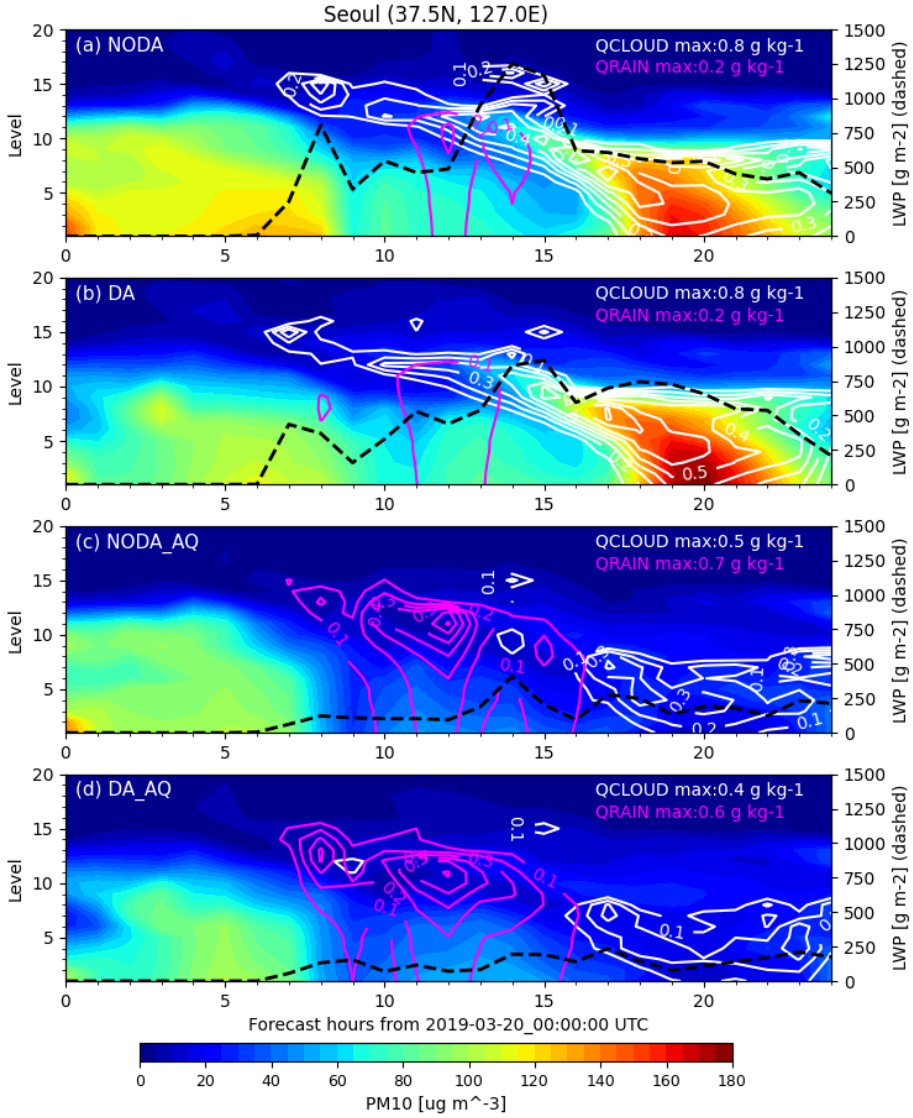
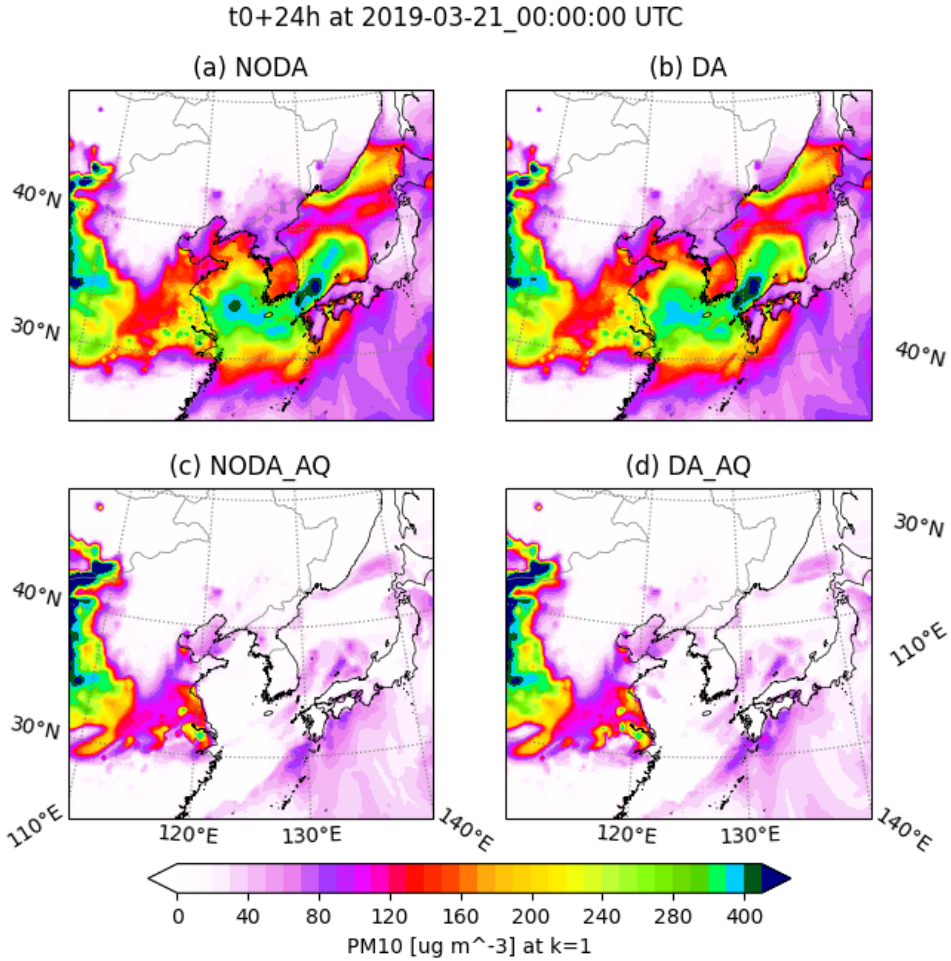


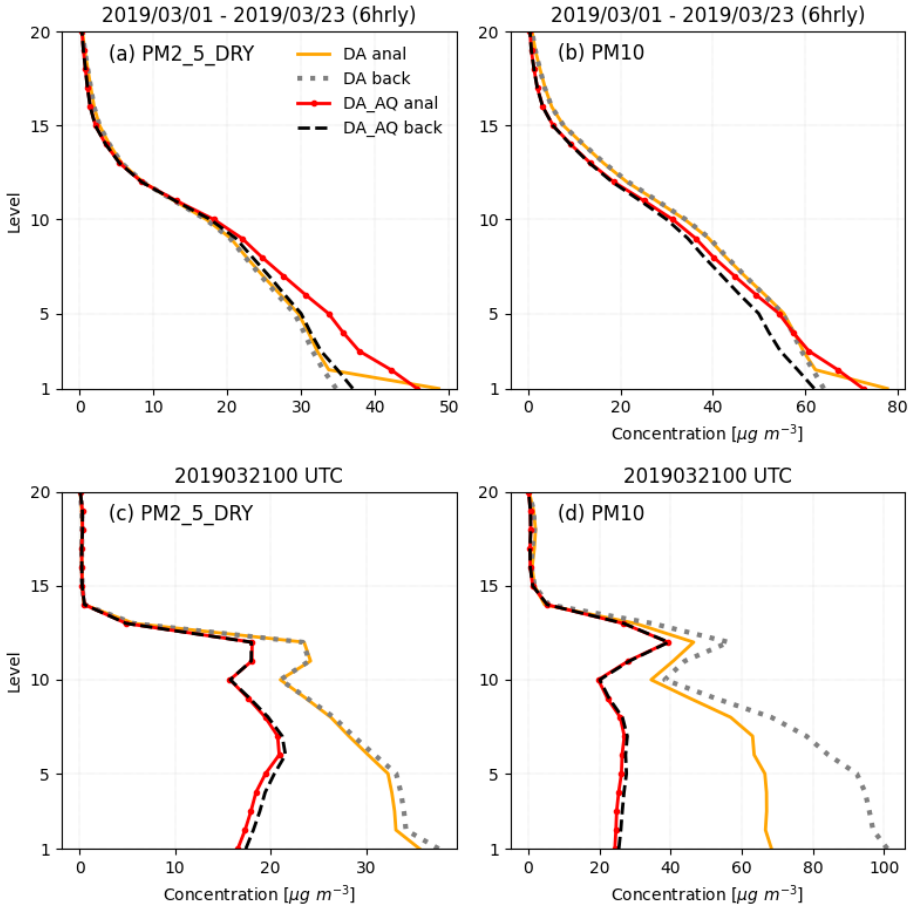
Figure 10. Time series of (top) surface $PM_{2.5}$ and (bottom) PM_{10} concentrations for three days (19-21 March 2019), averaged over 71 Korean verification sites (marked in Fig. 1b). In-situ observations (OBS; black triangle) are compared with cycling experiments for their 0-23 h hourly forecasts from the 00Z analysis every day. Gray dotted lines with the right y-axis are (top) mean sea level pressure (hPa) and (bottom) hourly rainfall (mm) observations averaged over 699 AWS sites over South Korea (marked in Fig. 1c.)



Time series of 0-24h forecasts of PM_{10} concentrations (colored) at Seoul, South Korea, in each experiment.
QCLOUD [g/kg]: white contours
QRAIN [g/kg]: pink contours
LWP [g/m2]: black dashed line w/ right y-axis

- Top two panels (w/o AQCHEM) produced large QCLOUD in the mid-troposphere at nighttime (around 12 UTC [21 KST]), followed by high PM_{10} concentration.
- With AQCHEM, bottom two panels simulated large QRAIN instead, leading to wet deposition of most aerosol particles.
- The formation and development of clouds (as simulated in LWP) are largely affected by aerosols in the aqueous phase.
- DA reduces the initial overestimation of PM concentrations.


t0+24h at 2019-03-21_00:00:00 UTC
(a) NODA
(b) DA
(c) NODA_AQ
(d) DA_AQ
40°N
30°N
110°E
120°E
130°E
140°E
0
40
80
120
160
200
240
280
400
PM10 [ug m^-3] at k=1


2019/03/01 - 2019/03/23 (6hrly)
(a) PM2_5_DRY
DA anal
DA back
DA_AQ anal
DA_AQ back
Level
Concentration [$\mu g\ m^{-3}$]
2019/03/01 - 2019/03/23 (6hrly)
(b) PM10
Concentration [$\mu g\ m^{-3}$]
2019032100 UTC
(c) PM2_5_DRY
Level
Concentration [$\mu g\ m^{-3}$]
2019032100 UTC
(d) PM10
Concentration [$\mu g\ m^{-3}$]

Summary

- ❑WRFDA V4.4 was expanded for the RACM-MADE-VBS-AQCHEM (chem_opt=109) to assimilate surface $PM_{2.5}$, PM_{10}, and four gas species (SO_2, NO_2, O_3, and CO); To be released in WRF V4.5.
- ❑In the WRF-Chem/WRFDA 3DVAR system, model error is not explicitly accounted for, but introducing aerosols in the aqueous phase in WRFDA seems beneficial in simulating wet removal of aerosols in cloudy conditions.
- ❑In the strong-constraint 3DVAR, reducing model errors through sophisticated physics mechanisms can make data assimilation more effective.
- ❑Aerosols interacting with clouds and radiation affected local weather conditions such as PBLH and 2-m temperature and RH (not shown).
- ❑With aqueous chemistry, sulfate aerosols in cloud water experience large increases, in association with low-level clouds over the Korean peninsula.

- ❑Limitations

i. A simple aqueous chemistry – may not work for mixed-phase clouds.

ii. Aerosol number concentrations are not included in the analysis.

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