Data assimilation of GEMS Aerosol Optical Depth (AOD) for operational air quality forecasting

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Satellite Aerosol Data Assimilation for NIER

- Project Goal
  - Establish the *real-time* assimilation capability of satellite AOD retrievals in the NIER operational air quality analysis and forecasting system (2023 – 2027)

- Key aspects
  - NSF NCAR develops an **online-coupled** atmosphere-chemistry analysis and forecast system for GEMS AOD
  - Simultaneous data assimilation of **multi-sensor, multi-channel AOD retrieval**s, along with available <u>meteorological</u> observations and <u>surface chemical</u> measurements ($PM_{2.5}$, PM_{10} , SO_2, NO_2, O_3, CO)
  - Use **advanced chemistry** parameterizations (RACM-MADE-VBS) with the latest version of **the full radiative transfer model** (e.g., CRTM) within the WRF-Chem/WRFDA 3DVAR (or hybrid DA) system
  - **Aerosol Optical Properties (AOPs)** are key to assimilating AOD and aerosol-radiation-cloud interactions.

Challenges in satellite aerosol data assimilation (DA)

Choice of control variables	• Too many gas and aerosol species with complex chemical reactions => How many of them do we really need for DA? • Meteorological fields (RH, T, Wind, etc.)
Choice of H(x) for AOD	• How can we compute the modeled AOD corresponding to retrievals? • Speed and complexity of a radiative transfer model (H(x)) • Large uncertainties in aerosol optical properties (AOPs) are the key
Treatment of Emissions forcing	• DA only updates initial conditions, but chemical transport models are constantly driven by emissions forcing after the initial time • Real-time updates through data assimilation
Evaluation against independent quantity	• Air Quality forecasts are validated against surface $PM_{2.5}$ or PM_{10} • AOD and PM are not prognostic; only diagnosed from aerosol mass conc. • AOD-PM relationship is not accounted in DA *per se*

Choice of control variables – how many aerosol species do we need for AOD DA?

Total no. of control variables in []

3D total mass conc. [1] — ECMWF IFS/4DVAR (Benedetti et al. 2009)

A subset of 3D aerosol species [1-7] — Major aerosol species from CMAQ/GSI (Kumar et al. 2019)

2D total column mass per size bin [3-8] — MOSAIC-8bin in WRF-Chem/GSI (Saide et al. 2013, 2014)

All 3D aerosol species defined in aerosol chemistry [14-70] — Mostly GOCART aerosols

[14-15] GOCART species in WRF-Chem/GSI (Liu et al. 2011; Schwartz et al. 2012; Ha et al. 2019)
=> [35] MADE-VBS in WRF-Chem/WRFDA (Ha 2022)
=> [70] MADE-VBS-AQCHEM in WRF-Chem/WRFDA (Ha et al. 2024)

Choice of observation operator (H(x)) for satellite AOD DA

- The Community Radiative Transfer Model (CRTM) provides the critical link between satellite radiances and physical properties of the atmosphere.
- CRTM can provide one of the most sophisticated ways to assimilate satellite Aerosol Optical Depth (AOD) retrievals.

Satellite Data Assimilation -> Analysis, Forecasting
Calibration / Validation
Satellite Simulations
Reanalysis
Real-time Weather Analysis / Support
Satellite Sensor Health Monitoring

Johnson et al. (2023)

Support for Polarized **UV, VIS/near-IR, IR, sub-MM, MW** – future: far IR. Instrument specific (center frequency, bandwidth, side bands, viewing geometry, polarization basis, spectral response)

Clouds: multi-species / habits supporting clouds / precipitation from VIS -> MW, microphysics-model specific LUTs (Thompson, GFDL, WSM-6)

Aerosols (salt, dust, smoke, black carbon, volcanic ash, etc.)

Gaseous species available in CRTM: H_2O, CO_2, O_3, N_2O, CO, CH_4, O_2, NO, SO_2, NO_2, HNO_3, N_2, OCS, and CFCs – *many others available from LBLRTM, not yet used in CRTM.*

Surface properties: land (soil moisture, vegetated), ocean (wind, foam,), sea-ice, snow cover (land, sea-ice, depth) --- primarily tested in IR/MW.

Active sensor development: space-based radar / lidar (backscat, extinct.)

Non-LTE (daytime) and Zeeman effects; Aircraft-based simulation

6

A schematic diagram of AOD DA

WRF-Chem simulation

Ambient Relative Humidity

Aerosol mass concentration for each species i (M_i)

Mean aerosol size for each mode m (r_e^m)

CRTM computation of optical properties for each aerosol species i with LUT (for pre-specified aerosol coefficients)

GEOS5-GOCART (19 species)

CRTM-AOD (Forward operator and Jacobian)

Satellite AOD retrievals (y^o)

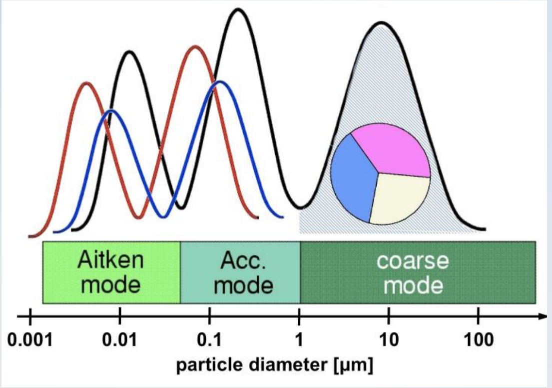
WRFDA (3DVAR)

Analysis (x^a)

$$x^a = x^b + PH(HPH^T + R)^{-1}(y^o - H(x))$$

$$J(x) = \frac{1}{2}\left(x - x^b\right)^T \mathbf{B}^{-1}\left(x - x^b\right) + \frac{1}{2}(y^o - H(x))^T \mathbf{R}^{-1}((y^o - H(x))$$

MADE-VBS (w/ 35 aerosol species) in three log-normal size distributions (Aquila et al. 2011)

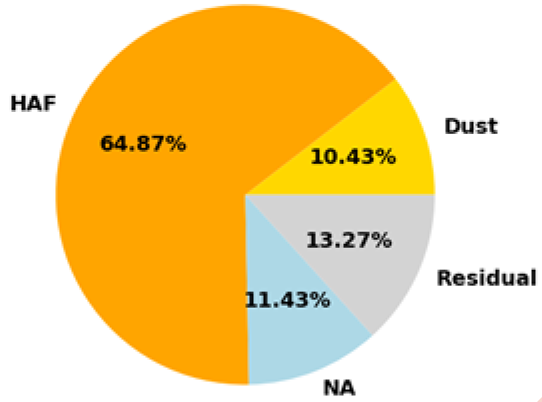


$H(x)$ for AOD:

$$\tau_\lambda = \sum_i^{N_i} \sum_k^{N_k} \beta_i^k(RH, \lambda, \rho_i, r_e) \cdot M_i^k \delta z$$

M_i is 3D mass concentration for i species [g/m^3],
δz the layer thickness[m]
β_i mass extinction coefficient for each species i

Optical aerosol species for AOD assimilation => Large discrepancies



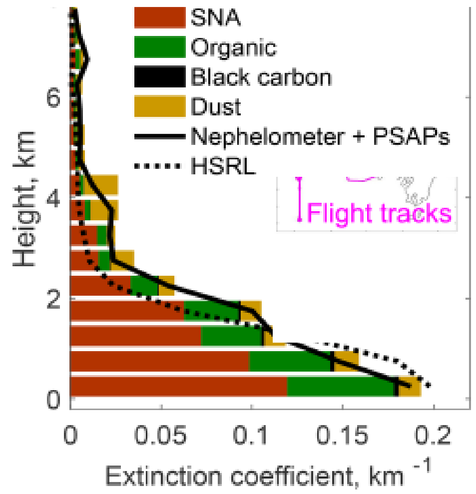
GEMS ATBD

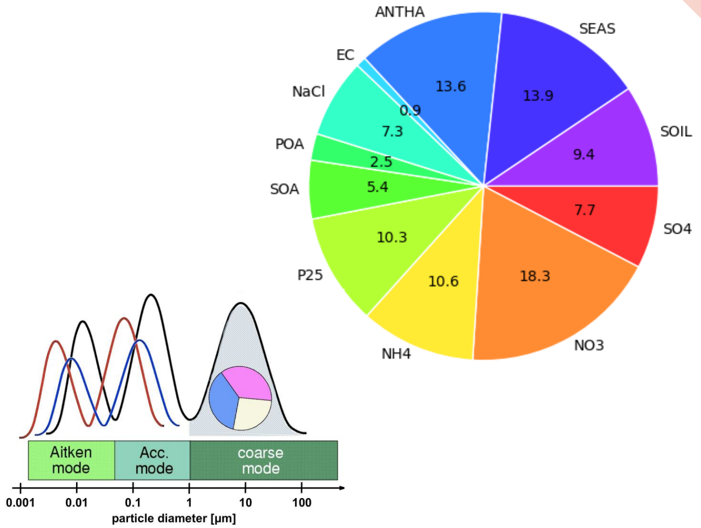
High-Absorbing Fine (OC, BC; 65%), Non-Absorbing (Inorganic; 11%), Dust (10%)

Observation

Sulfate-Nitrate-Ammonium (59%), Organic (27%), Dust (12%)

KORUS-AQ (Zhai et al.2021)





WRF-Chem

MADE-VBS

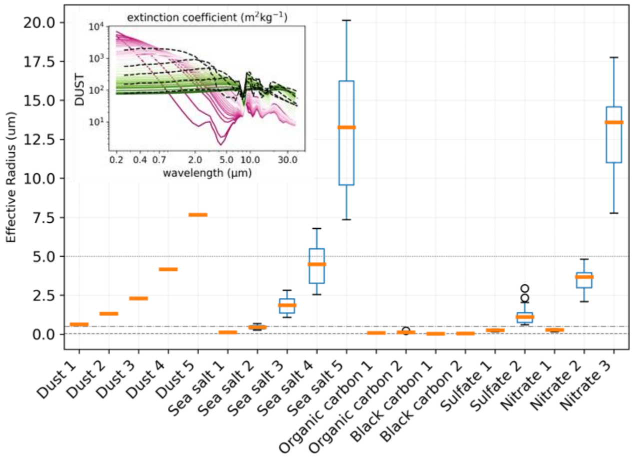
35 species in three size modes

Internally mixed within each mode

CRTM

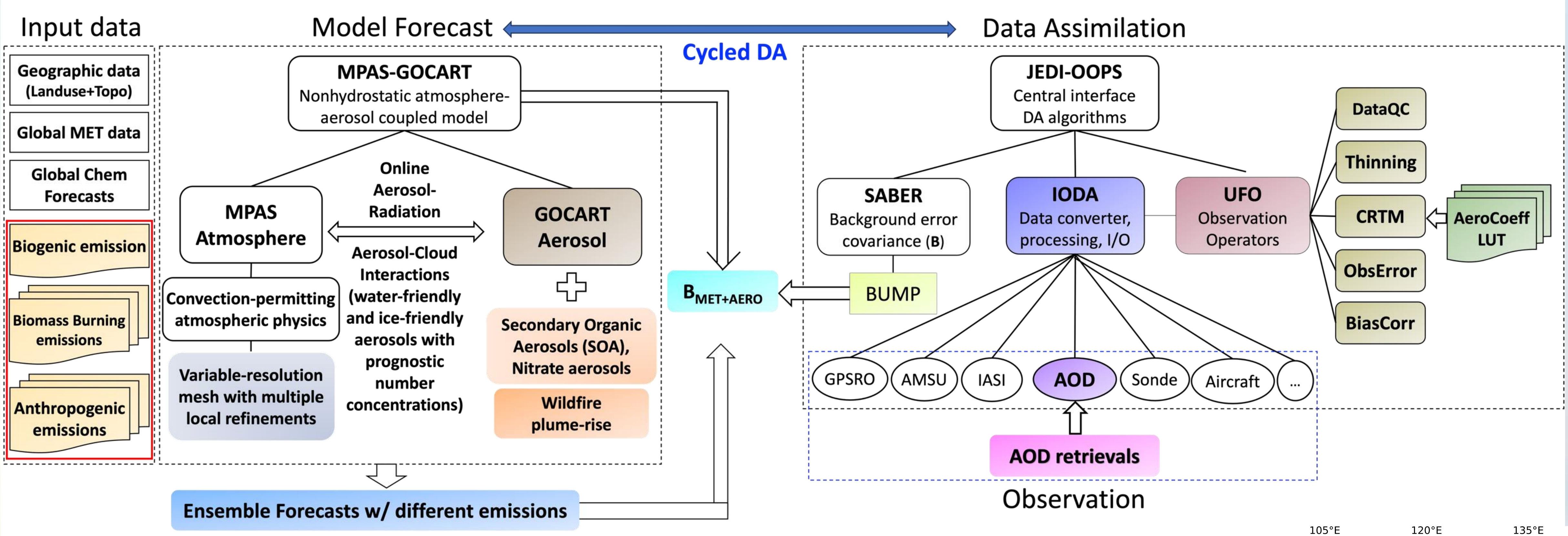
19 GOCART-GEOS5 species

Externally mixed

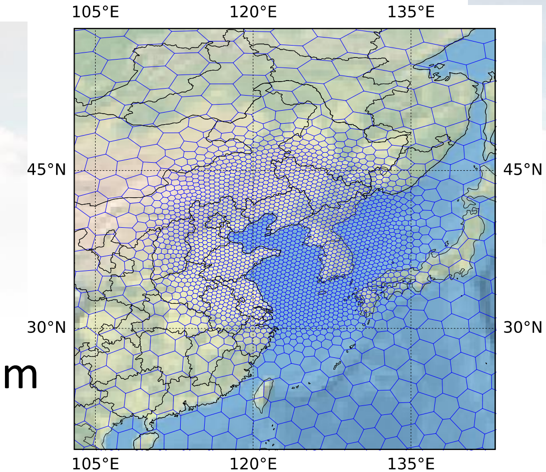


Substantially different assumptions of atmospheric constituents => systematic bias

NSF NCAR next-generation chemical weather system using MPAS-JEDI



- Joint Effort for Data assimilation Integration (JEDI) for an online-coupled MPAS-GOCART model
- A unified DA system using variable-resolution global/regional meshes
- Advanced DA techniques available for aerosol+tracers+cloud+emission analysis
- Assimilating weather and chemical observations including all-sky radiances and AOD retrievals from NASA PACE AOD (w/ new devs in colored boxes); easily extensible for TEMPO and GEMS AOD



Concluding remarks

- Geostationary satellites provides invaluable information on the upstream flow.
- Multi-sensor, multi-channel retrievals/radiances need be assimilated together.
- **Data processing and validation, and model evaluation should all be conducted within the data assimilation framework (for consistency and systematic changes).**
- **Actionable science can only be achieved through multi-project and multi-agency efforts.**

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