Evaluation of Aerosol Characterizations in Numerical Weather Modeling for Emerging DoD Technologies and Climate Change Studies

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Overview

Abstract: This research evaluates atmospheric aerosols characterized by the Weather Research and Forecasting with Chemistry (WRF-Chem) model using the Goddard Chemistry Aerosol Radiation and Transport (GOCART) aerosol scheme option and the Global Aerosol Data Set (GADS).

Research Objectives

1. Identify a method to derive radiative transfer solutions at any wavelength or spectral band (via GADS and LEEDR) using aerosol data from numerical weather prediction (NWP)

2. Identify why tracking aerosol number concentration may be better for directed energy, radiative transfer, and cloud/precipitation microphysics

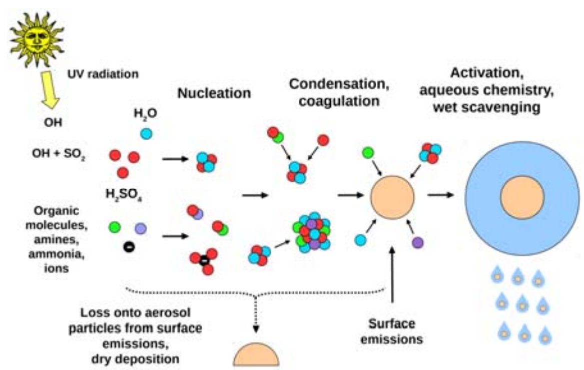
3. Identify a method to obtain aerosol number concentration from numerical weather prediction (NWP) models, particularly WRF-Chem v3.8.1, from the PM2.5 mass densities

4. Identify methods to bring the NWP PM2.5 derived number concentrations more in line with the measurements

Model Assumptions

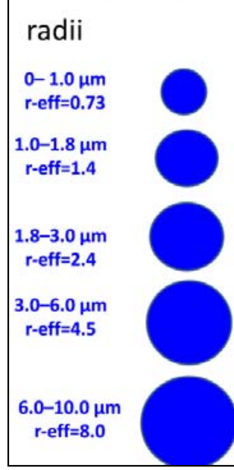
GOCART

- WRF-Chem models dynamic changes in the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology
- The Goddard Chemistry Aerosol Radiation & Transport (GOCART) model is a bulk aerosol model
  - Simulates major tropospheric aerosol types and evolution: sulfate, dust, black carbon and organic carbon, and sea-salt emissions
  - Mass concentration ($\mu g/m^3$) outputs
  - Radiative properties from Mie theory with refractive indices from Barnard et al – ties to the Global Aerosol Data Set (GADS)
  - Does not consider secondary organic aerosols, specifically water soluble (WASO)
- Aerosol schemes similar to GOCART to be used in NWP:
  - Coupled Large-scale Aerosol Simulator for Studies in Climate (CLASSIC)
  - Next Generation Unified Forecast System (USF)



Distribution A

Dust Size Bins in WRF-Chem



Dust in WRF-Chem is distributed into 5 size bins:

Type	reff_dust(μm)	Density(g cm-3)
bin1	0.73	2500
bin2	1.4	2650
bin3	2.4	2650
bin4	4.5	2650
bin5	8	2650

- $PM_{2.5}$=bin1+0.3125*bin2
- PM_{10}=bin1+bin2+bin3+0.87*bin4

Model Assumptions

GOCART

Table 1. Assumed densities and refractive indices ($n + ik$) of the indicated species. Unless otherwise noted, the refractive indices are for a wavelength of 870 nm.

species	Density (g/cm^3)	Refractive index (real), n	Refractive index (imaginary), k
SO_4	1.8	1.52	0
NO_3	1.8	1.5	0
NH_4	1.8	1.5	0
Cl	2.2	1.45	0
Na	2.2	1.45	0
Ca	2.6	1.56	0
Mg	1.8	1.5	0
Organic Matter (OM) (Kanakidou et al., 2005; refractive index range is 300 nm to 800 nm)	1.4	1.45	0
Elemental Carbon (EC) (Bond and Bergstrom, 2006; refractive index for 550 nm)	1.8	1.85	0.71
Dust (Prasad and Singh, 2007; Mishra and Tripathi, 2008)	2.6	1.55	0.002
water	1.0	1.33	0.0

Assumptions made:

1. Aerosols are spheres.
2. Spectral refractive index for each species must be assigned.
3. The density of each species
4. Hygroscopic growth factor (GF)
5. The combo of calculated optical properties with mixing state assumption

Uncertainties:

1. Bias in aerosol type concentrations
2. Hygroscopic aerosols and rate of change in particle's radius with RH
3. Spatial distribution of aerosol mass within the particle matter for optical properties

SOURCE: Barnard et al., 2010: Technical Note: Evaluation of the WRF-Chem "Aerosol Chemical to Aerosol Optical Properties" Module using data from the MILAGRO campaign. Atmos. Chem. Phys., 10, 7325–7340. doi:10.5194/acp-10-7325-2010

Model Assumptions
GADS

- The Global Aerosol Data Set (GADS) is a global aerosol climatology
  - Consists of 10 aerosol components, with individual particle size distributions
  - Horizontal resolution is 5x5-degree with seasonal variations (summer, winter)
  - Number concentration (particles/cm^{-3}) outputs
  - Radiative properties from Mie theory and refractive indices for 200 nm to 40 µm

As size distributions, lognormal distributions [cf., e.g., Deepak and Gerber (1983)] are applied for each component *i*:

$$\frac{dN_i(r)}{dr} = \frac{N_i}{\sqrt{2\pi}\, r \log\sigma_i \ln 10} \exp\left[\frac{1}{2}\left(\frac{\log r - \log r_{\mathrm{mod}\,N,i}}{\log\sigma_i}\right)^2\right],$$

Table 1c. Microphysical properties of aerosol components in dry state. Here, σ, r_{modN}, r_{modV}, r_{min}, and r_{max} are parameters of the lognormal size distributions (see section 3c). The term ρ is the density of the aerosol particles and M^* is the aerosol mass per cubic meter air, integrated over the size distribution and normalized to 1 particle per cubic centimeter of air. The term M^* [(μg m^{-3}) (particles cm^{-3})$^{-1}$] is calculated with a cutoff radius of 7.5 μm.

Component	File name	σ	r_{modN} (μm)	r_{modV} (μm)	r_{min} (μm)	r_{max} (μm)	ρ (g cm^{-3})	M^* (μg m^{-3})/(part. cm^{-3})
Insoluble	INSO	2.51	0.471	6.00	0.005	20.0	2.0	2.37E1
Water-soluble	WASO	2.24	0.0212	0.15	0.005	20.0	1.8	1.34E−3
Soot	SOOT	2.00	0.0118	0.05	0.005	20.0	1.0	5.99E−5
Sea salt (acc. mode)	SSAM	2.03	0.209	0.94	0.005	20.0	2.2	8.02E−1
Sea salt (coa. mode)	SSCM	2.03	1.75	7.90	0.005	60.0	2.2	2.24E2
Mineral (nuc. mode)	MINM	1.95	0.07	0.27	0.005	20.0	2.6	2.78E−2
Mineral (acc. mode)	MIAM	2.00	0.39	1.60	0.005	20.0	2.6	5.53E0
Mineral (coa. mode)	MICM	2.15	1.90	11.00	0.005	60.0	2.6	3.24E2
Mineral-transported	MITR	2.20	0.50	3.00	0.02	5.0	2.6	1.59E1
Sulfate droplets	SUSO	2.03	0.0695	0.31	0.005	20.0	1.7	2.28E−2

- **Insoluble** – consists mostly of soil particles with a certain amount of organic material
- **Water-soluble** – originates from gas to particle conversion; consists of various kinds of sulfates, nitrates, and other organic substances; contains more than sulfates
- **Soot** – represents absorbing black carbons
- **Sea Salt** – various kind of salt contained in seawater; two modes allow for different wind-speed-dependent particle sizes
- **Minerals** – includes desert dust; mixture of quartz and clay with 3 modes
- **Transported Minerals** – desert dust transported over long distances
- **Sulfate** – describes the amount of sulfate found in the Antarctic region

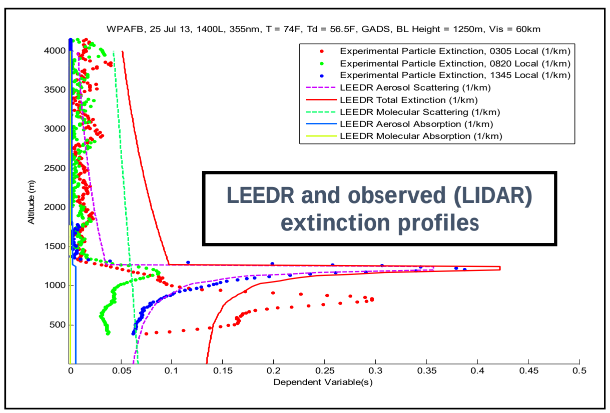
Laser Environmental Effects Definition & Reference

Objective #1 – Radiative Transfer Solutions for any Wavelength/Band

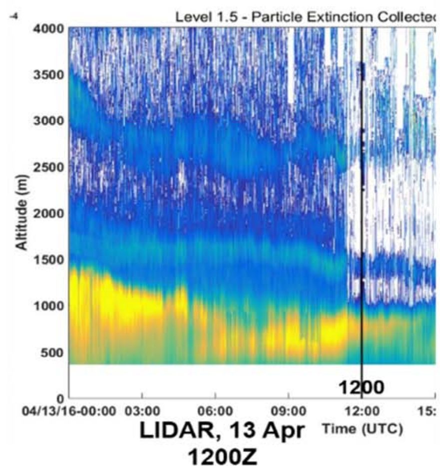
LEEDR

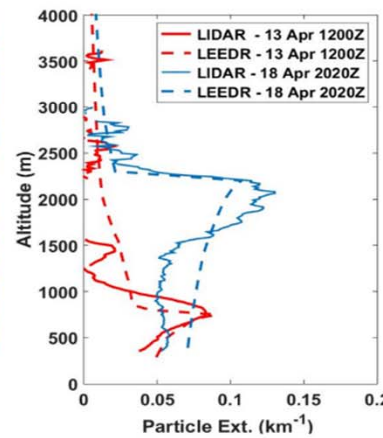
Laser Environmental Effects Definition and Reference

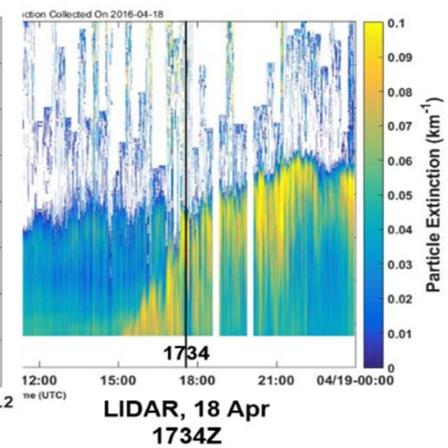
Characterizes effects from 200 nm to 8.6 meters



Vertical Aerosol Extinction Profiles







Laser Environmental Effects Definition & Reference

Objective #1 – Radiative Transfer Solutions for any Wavelength/Band

- Atmospheric characterization and radiative transfer code that calculates line-by-line and spectral band solutions by creating correlated, physically realizable profiles of meteorological and environmental effects (e.g. gaseous and particle extinction, optical turbulence, and cloud free line of sight) data

- Accesses terrestrial and marine atmospheric and particulate climatologies
  - Graphical access to and export of probabilisitc data from the Extreme and Percentile Environmental Reference Tables (ExPERT)

LEEDR
Laser Environmental Effects Definition and Reference

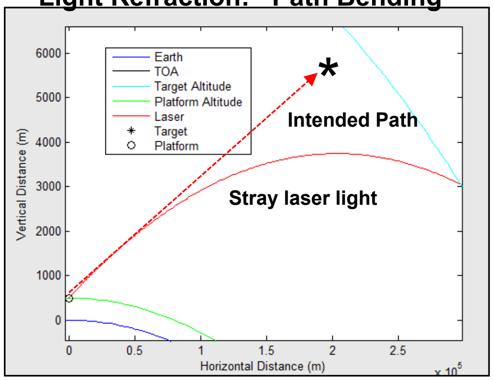
Characterizes effects from 200 nm to 8.6 meters

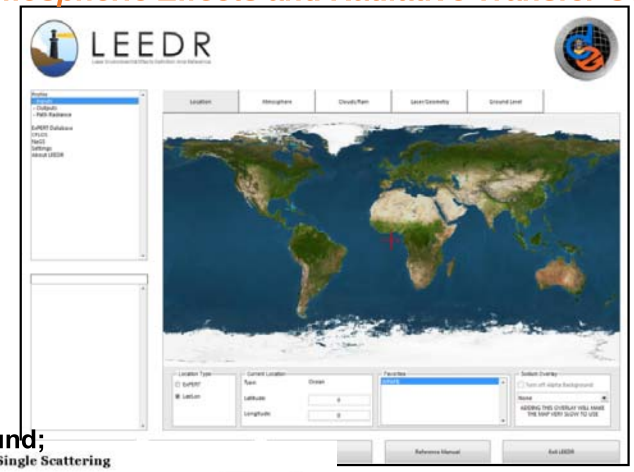
Laser Environmental Effects Definition & Reference

Objective #1 – Radiative Transfer Solutions for any Wavelength/Band

V&V'd Atmospheric Effects and Radiative Transfer Code for HEL

Light Refraction: Path Bending

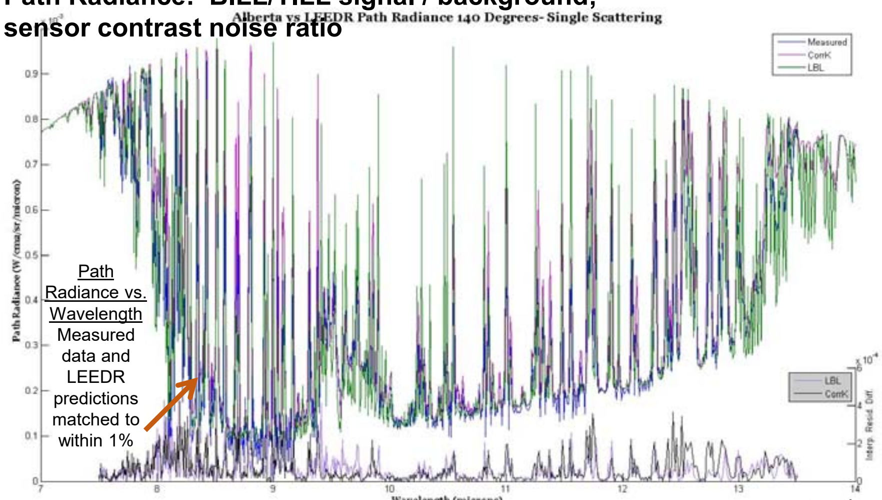




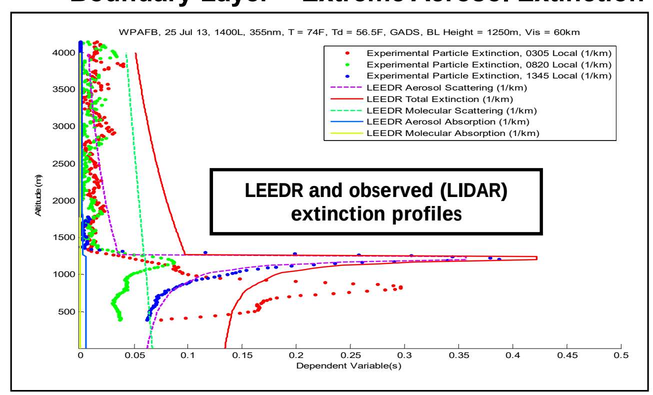
Creates physically realizable horizontal / vertical profiles of meteorological and weather event data and associated radiative effects (e.g. optical extinction, path radiance):

- Aerosol and surface observation (i.e. T, P, RH) climatology at 573 ExPERT and 1° x 1° oceanic grid locations
- Numerical weather forecast, re-analysis data
- Profiles optical turbulence (i.e. C_n^2)
- Accounts for light-refraction and single/multi-scatter
- Includes sun-moon calculator

Path Radiance: BILL/TILL signal / background; sensor contrast noise ratio



Boundary Layer - Extreme Aerosol Extinction

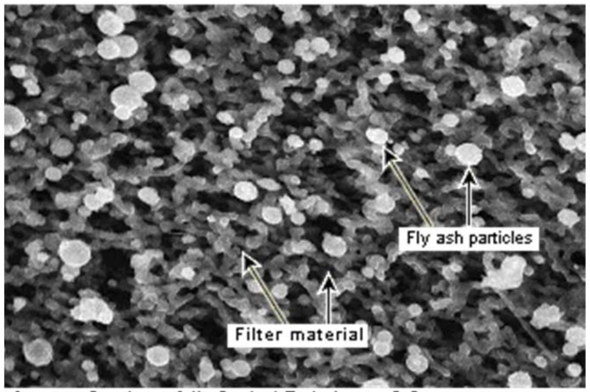


Distribution A

Mass to Number Concentration

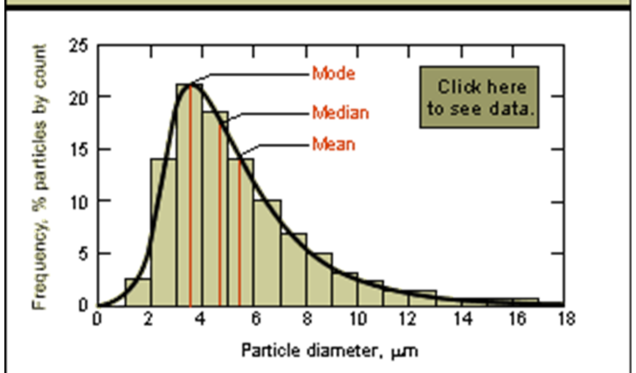
LEEDR Aerosol Equations

Figure 1. Photomicrograph of Fly Ash Particles on an MCE Filter



Source: Courtesy of Air Control Techniques, P.C.

Figure 2. Histogram of a Particle Size Distribution



Source: *Particle Size Analysis in Industrial Hygiene*, Academic Press, 1971.

The distribution (lognormal)

$$\frac{dN(r)}{d(\log r)} = \frac{N}{(2\pi)^{1/2}\log(\sigma)}\exp\left[-\frac{(\log r - \log r_M)^2}{2(\log \sigma)^2}\right]$$

The Mie Extinction

$$\beta_{e,s,a}(\lambda) = \int_{r_1}^{r_2} Q_{e,s,a}(n,\lambda,r)\pi r^2 \frac{dN(r)}{r\ln 10\, d(\log r)}dr$$

$$\approx \sum_{i=r_{\min}}^{r_{\max}} Q_{e,s,a}(n,\lambda,r_i)\pi r_i^2 \frac{dN_i}{r_i \ln 10\, d(\log r_i)}\Delta r_i$$

The water uptake size adjustment

$$\log(a_w) = \pm\left[-\ln\left(ND\sqrt{2\pi}\log\sigma\right)2\,(\log\sigma)^2\right]^{1/2} + \log r_M$$

The refractive index adjustment

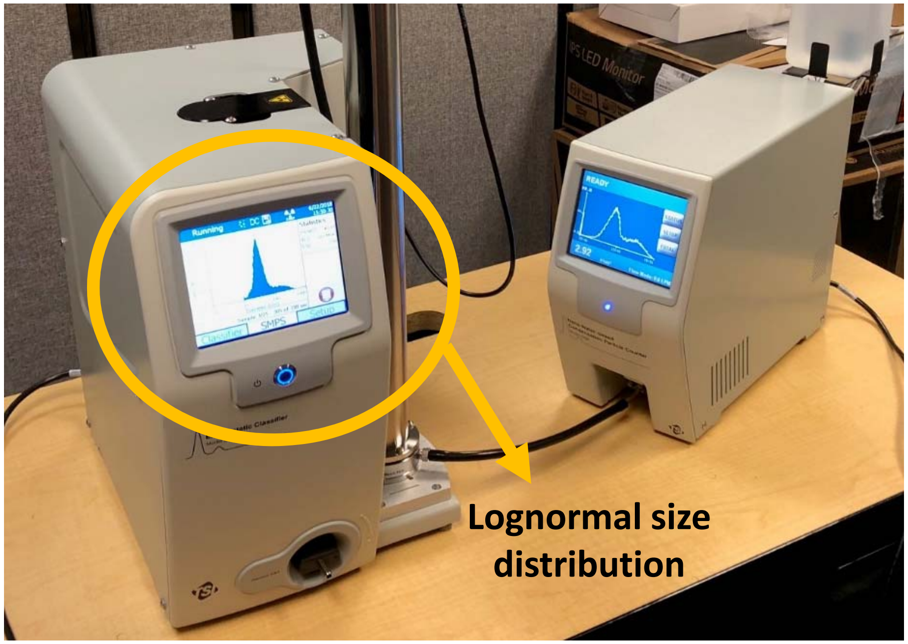
$$n = n_w + (n_0 - n_w)\left[\frac{r_0}{r(a_w)}\right]^{3}$$

Mass to Number Concentration

Objective #2 – Number Density Better for DE & Radiative Transfer?

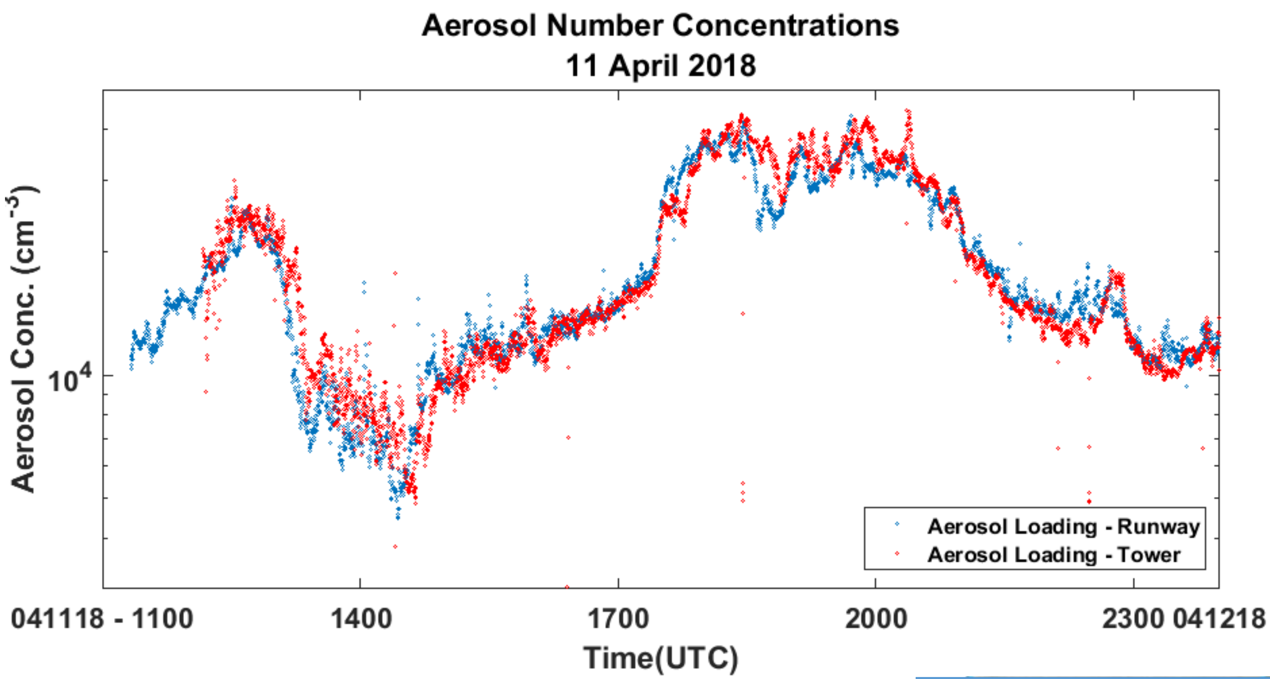
- **Mass Concentration**
  - Legacy method
  - Much easier to validate mass densities rather than number concentrations
  - Mass concentration requires assumptions about the size distribution (lognormal)

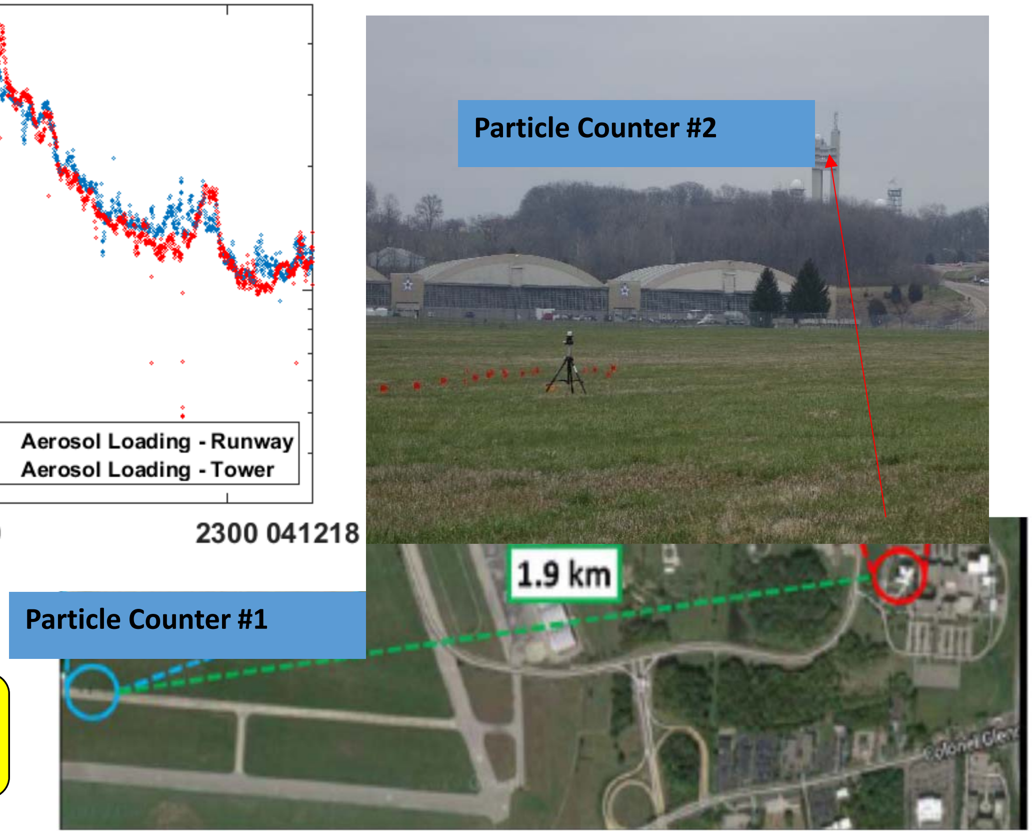
- **Number Concentration**
  - Directly used in Mie theory calculations to calculate scattering, absorption, extinction coefficients
  - Used in numerical model microphysical schemes – more accurate cloud and precipitation development
  - Visibility calculations based on number density
  - Sparse measurements characterize regional analysis
  - Number concentration requires assumptions about particle types



Mass to Number Concentration

Objective #2 – Number Density Better for DE & Radiative Transfer?





Aerosol loading can be characterized by sparse particle counting network

Mass to Number Concentration

Objective #3 - Conversion Methodology

Total mass of particles/cm^3, dM_i, in any size bin "i" can be expressed as:

$$dM_i = dN_i * m_i$$

$$dM_i = dN_i * \rho_i V_i$$

$$dM_i = dN_i * \rho_i * \frac{4}{3}\pi r_i^3$$

$$dN_i = \frac{dM_i}{\rho_i * \frac{4}{3}\pi r_i^3}$$

where

dM_i = mass concentration in size bin "i" ($\mu g / m^3$) – WRF_CHEM output units
dN_i = number concentration in size bin "i" (cm^{-3}) – LEEDR units
m_i = effective mass of each individual particle in bin "i" – (g)
ρ_i = effective density of each individual particle in bin "i" – (g / cm^3)
V_i = effective volume of each individual particle "i" – (cm^3)
r_i = Effective particle radius of each individual particle in bin "i" (Geometric midpoint of particle size channel) – (μm)

Species	Abbreviation	Density (g/cm^3)	Effective Radius (microns)
Sulfate	Sulf	1.8	0.399
Black carbon 1	BC1	1.8	0.039
Black carbon 2	BC2	1.8	0.039
Organic carbon 1	OC1	1.4	0.087
Organic carbon 2	OC2	1.4	0.087
Other PM2.5	p25	2.65	1.4
Other PM10	p10	2.65	4.5
Dust - Size Bin 1	Dust1	2.5	0.73
Dust - Size Bin 2	Dust2	2.65	1.4
Dust - Size Bin 3	Dust3	2.65	2.4
Dust - Size Bin 4	Dust4	2.65	4.5
Dust - Size Bin 5	Dust5	2.65	8.0
Sea Salt – Size Bin 1	Seas1	2.2	0.3
Sea Salt – Size Bin 2	Seas2	2.2	1.0
Sea Salt – Size Bin 3	Seas3	2.2	3.25
Sea Salt – Size Bin 4	Seas4	2.2	7.5

GOCART particle density and effective radius assumptions

Mass to Number Concentration

Evaluating PM2.5

- PM2.5 is considered planetary boundary layer aerosols
- Mass to Number Concentration conversions are applied to each aerosol species (type, size bin) output
- GOCART provides a diagnostic output of Total PM2.5 Dry value using the following equation:

Total PM2.5 Dry = SUM(p25, BC1, BC2, OC1, OC2, Dust1)
+ 0.286 * (Dust2)
+ Seas1
+ 0.942 * (Seas2)
+ Sulf * (nh4_mfac)
+ (OC1 + OC2) * (oc_mfac)

Objective #4

Already noted that GOCART does not consider water-soluble aerosols

- Due to known deficiencies in sulfates and organic carbons, scalers are used to increase these values for the PM2.5 Dry output ***in GOCART post-processing routines***.
  - nh4_mfac = 1.375 to account for missing Sulfate mass
  - oc_mfac = 0.8 to account for Carbon to Organic mass

Modeled vs Measured

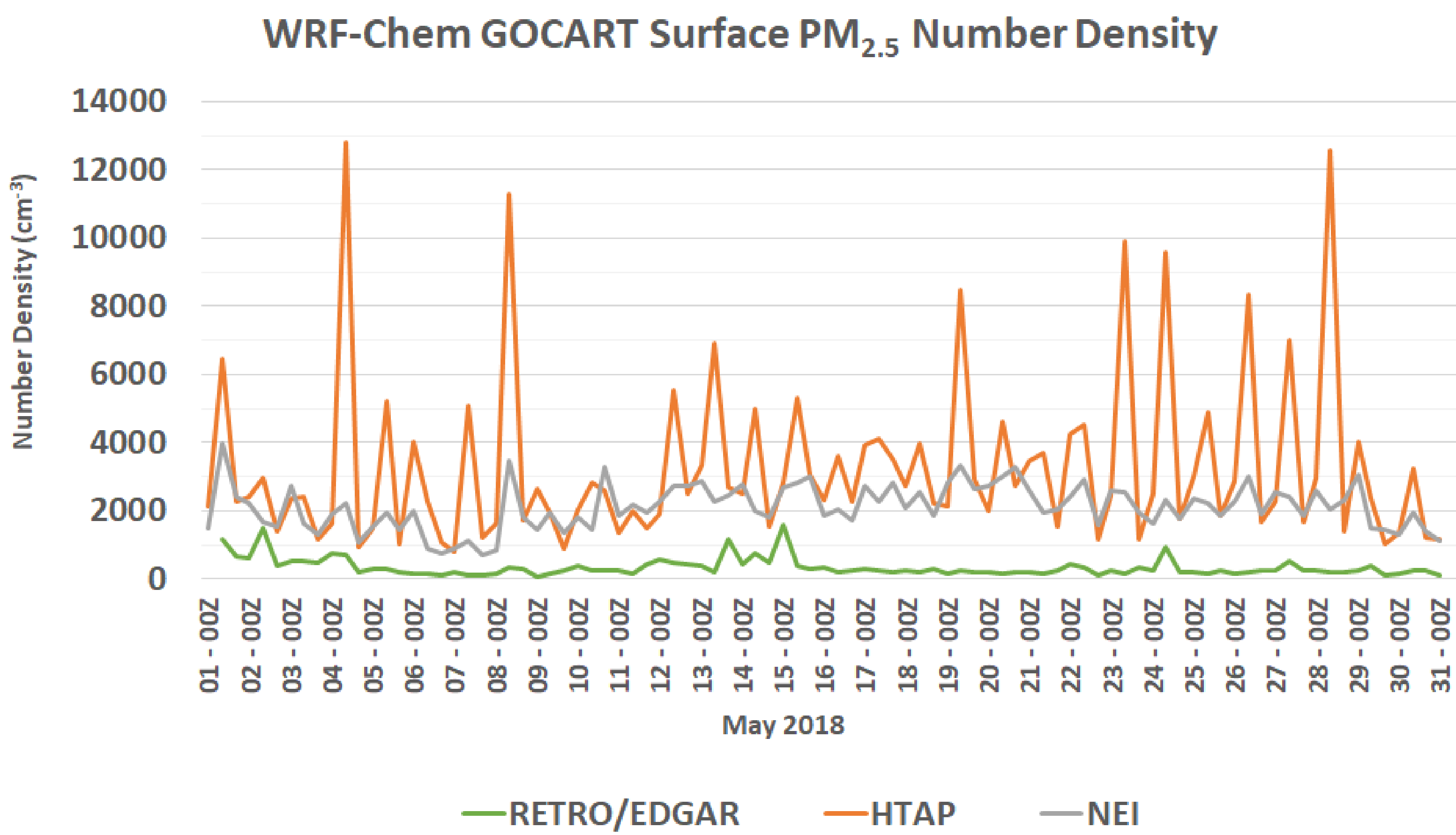
WRF-Chem Data Sets

- WRF-Chem data was generated for a CONUS domain, covering 1-31 May 2018. The following aerosol emissions databases were used to initialize the model:
  1. RETRO-EDGAR – global gridded data sets for anthropogenic emissions, course resolution
  2. EDGAR-HTAP –Hemispheric Transport of Air Pollution regional emissions, 10km resolution
  3. NEI-2011 – gridded, hourly CONUS emissions from the EPA emissions programs, 4km resolution

- Results at Dayton, OH site evaluated for 3 TODs
  - 1200 UTC – Model initialization for the meteorology was provided by the Global Air-Land Weather Exploitation Model (GALWEM), a product of the USAF 557th Weather Wing
  - 1800 UTC – 6-hour forecast
  - 0000 UTC –12-hour forecast
    - Note that anthropogenic surface and point source aerosols were updated hourly, and the chemistry was cycled back into the model from previous 24-hour forecast.

Modeled vs Measured

GOCART Results from Various Emissions Databases



Distribution A

Modeled vs Measured

Real-Time Aerosol Measurements

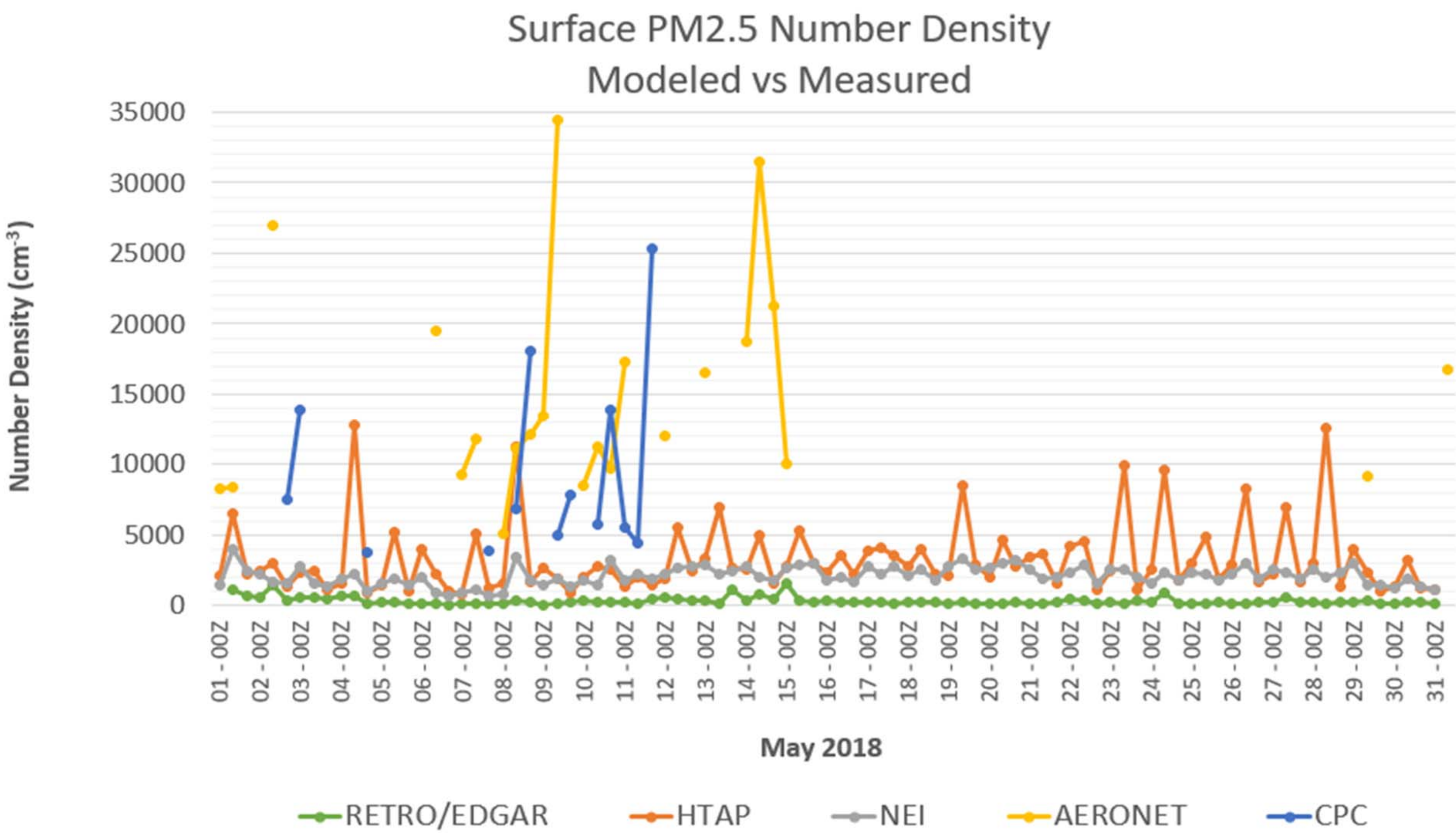
- Only need apply a handful of passive techniques to largely describe actual aerosol loading / optical effects
  - **Sun Photometer**
    - Leads to multi-wavelength aerosol optical thickness using Beer-Bouguer law
    - From visibility the aerosol loading can be computed
  - Visibility
    - Use Koschmeider and Beer-Lambert laws to deduce total aerosol extinction
    - A more quantitative way to get aerosol loading
  - **Particle counter somewhere along path**
    - Day/night aerosol concentration (and size distribution)
    - Surface measurement readily leads to vertical concentration profile throughout well-mixed boundary layer

GADS Aerosols Eglin Summer				
Sea Salt (ACC) (cm^-3)	Sea Salt (COA)	Soot	Water-soluble	Insoluble
6.994	0.0008224	3599	4044	0
Continental Polluted				
Sea Salt (ACC) (cm^-3)	Sea Salt (COA)	Soot	Water-soluble	Insoluble
0	0	34300	15700	0.6

17		
18	Time	Conc (#/cm³)
19	8:30:09	10000
20	8:30:19	10500
21	8:30:29	10400
22	8:30:39	10200

Modeled vs Measured

GOCART Results from Various Emissions Databases



Distribution A

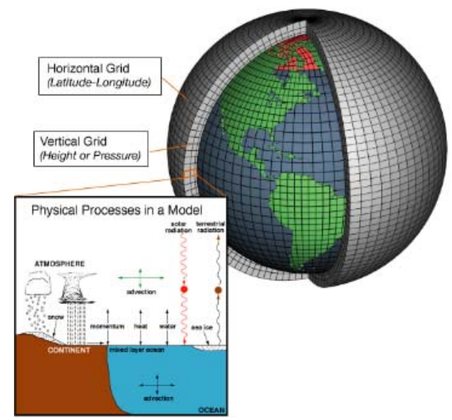
Modeled vs Measured

Objective #4 - Methods to Improve NWP Aerosol Modeling

- Incorporating GADS' water soluble aerosols into WRF-Chem initialization will fill the current void

- Preliminary results show that initializing WRF-Chem with HTAP emissions simulates PM2.5 number concentrations that are more in-line with measurements
    - Determine appropriate scaler to increase known deficiencies in PM2.5 values

- Enhance NWP models by incorporating point source measurements
    - Particle counts, sun photometers included in standard MET observations
    - Improve aerosol forecast capability, impacts of aerosol on radiation, microphysical processes
    - Allow NWP models' microphysical and cloud parameterization schemes to use predicted aerosols
    - Addition of aerosols in NWP modeling has a potential to improve global precipitation distribution and cloud properties – direct impact on climate studies



Summary

Research Objectives:

1. Identified a method to derive radiative transfer solutions at any wavelength or spectral band (via GADS and LEEDR) using aerosol data from numerical weather prediction (NWP)

2. Discussed why tracking aerosol number concentration may be better for directed energy, radiative transfer, and cloud/precipitation microphysics

3. Identified a method to obtain aerosol number concentration from numerical weather prediction (NWP) models, particularly WRF-Chem v3.8.1, from the PM2.5 mass densities

4. Identified methods to bring the NWP PM2.5 derived number concentrations more in line with the measurements

Future Work

- Validate the assumption of a lognormal size distribution and 2km scale height
- Incorporate GADS' water soluble aerosols into WRF-Chem GOCART
- Determine the regional and seasonal organic carbon scaling factors
  - Apply machine learning techniques (similar to MOS or model output statistics)
  - Longer periods of time need to be evaluated for different regions where data is available
- Investigate correlations between diurnal PM2.5 number densities, human activity, and turbulence
- Leverage surface aerosol concentrations via particle counters capturing ultra-fine/fine aerosol effects to improve reported visibility (e.g. greater than 10 SM)
- Ultimately, enhance NWP models by incorporating point source measurements