Assessment of Improved WRF-Chem $PM_{2.5}$ Characterization via Implementation of an Aerosol Measurement Network

1st Lieutenant Daniel Jagoda

Dr. Steven Fiorino

Dr. Steven Peckham

Dr. Kevin Keefer

Jaclyn Schmidt

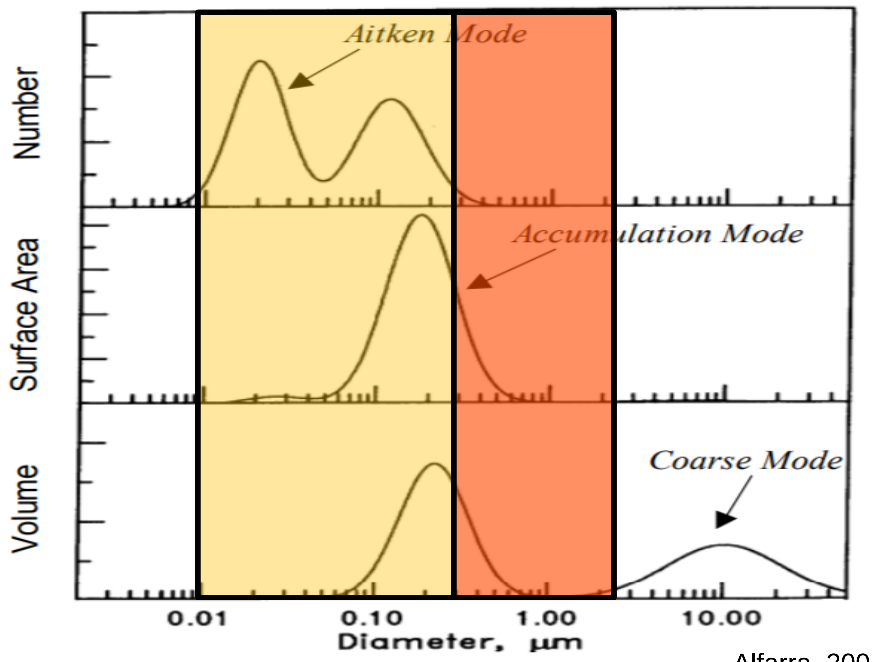
12-16 Jan 2020

Research Objectives

1. Establish $PM_{2.5}$ meteorological relevance
2. Expose non-standardization in aerosol measurement community
3. Improve WRF-Chem characterization with real-time data
4. Develop a method to introduce $PM_{2.5}$ to observational meteorology

Background

- Atmospheric Composition
  - $PM_{2.5}$ (1-nm to 2.5-µm)
    - Cloud Condensation Nuclei
    - Light Extinction
    - Health Hazards
  - Number (cm^{-3}) vs Mass ($\mu g/m^3$)



Alfarra, 2004

- Numerical Weather Prediction (NWP)
  - Emissions Inventories vs Real-Time Observation

- Operational Weather
  - Horizontal Visibility Observations

Visibility > 10 Statute Miles
"UNRESTRICTED"

Plan of Attack

WRF-Chem

1 Mar - 30 Apr 2019
Runs Start @ 00Z
Forecasts +48-hrs

$PM_{2.5}$ Observation

Particle Counter
2.5-nm Detection
Hourly Averages

TSI, 2018

Modified WRF-Chem

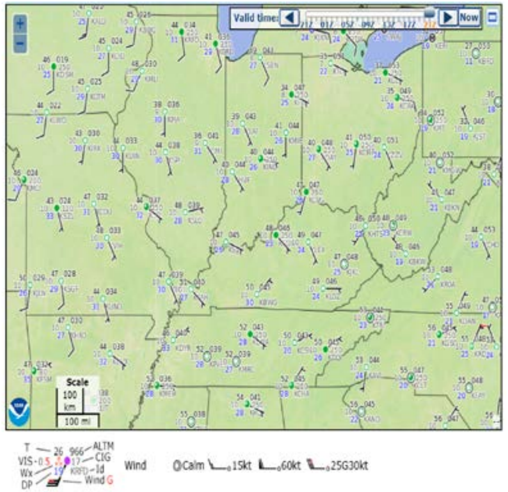
Standard Emissions
Point Initialization
Mass Conversion

$$N = \frac{M}{\rho_M * \frac{4}{3}\pi r_M^3}$$

N = *number concentration* (cm^{-3})
M = *mass density* (µg/m^3)
ρ_M = *median density* (g/cm^3)
r_M = *median radius* (µm)

Sustain Observation

Real-Time Network
Leverage METAR
Advanced Visibility

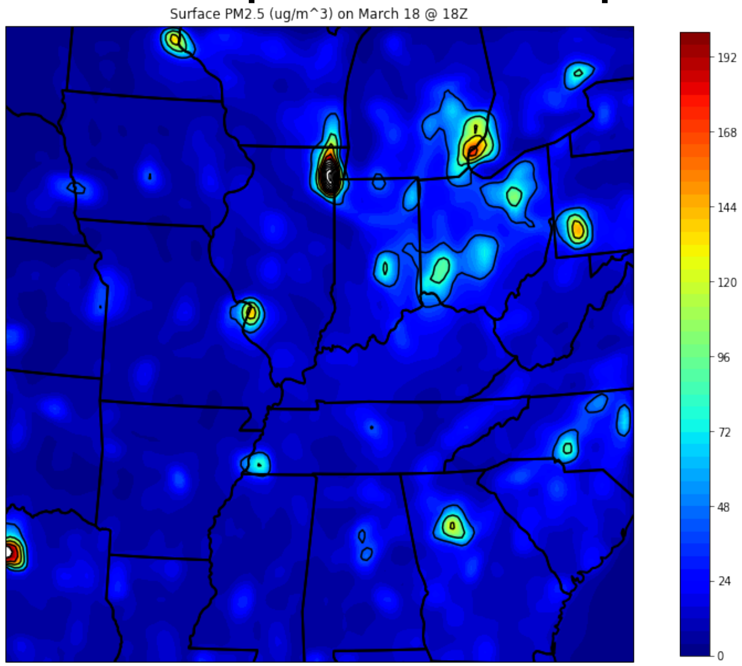


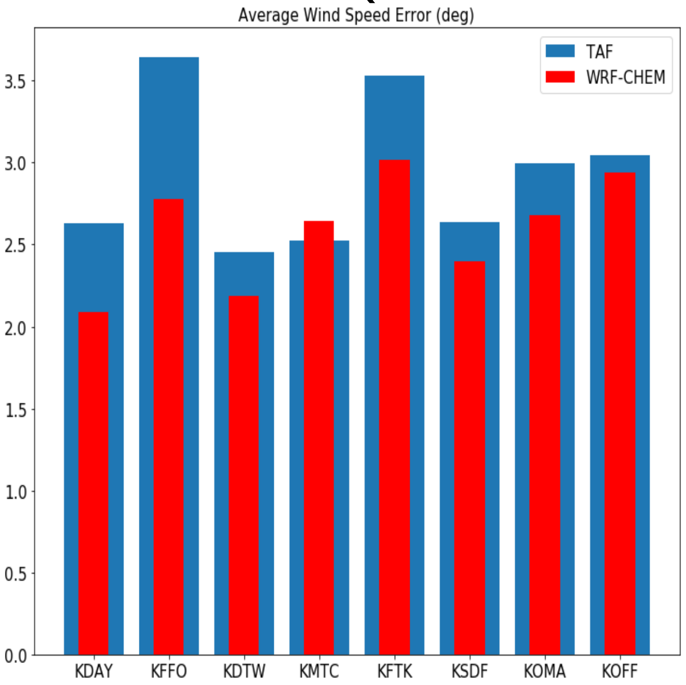
AWC, 2020

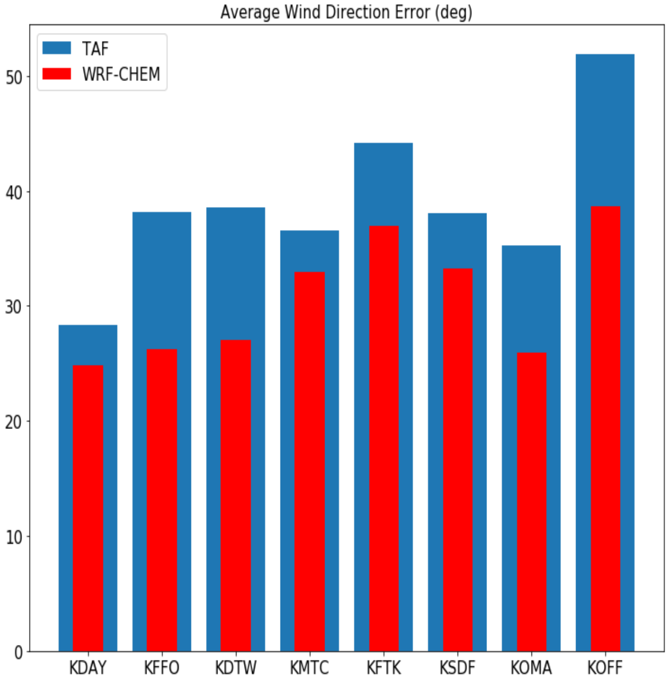
WRF-Chem

- Tested for Meteorological Accuracy
- Goddard Chemistry Aerosol and Radiation Transport (GOCART)
  - Lognormal Size Distribution
- Emissions Inventory

Hemispheric Transport of Air Pollution (HTAP, 2017)



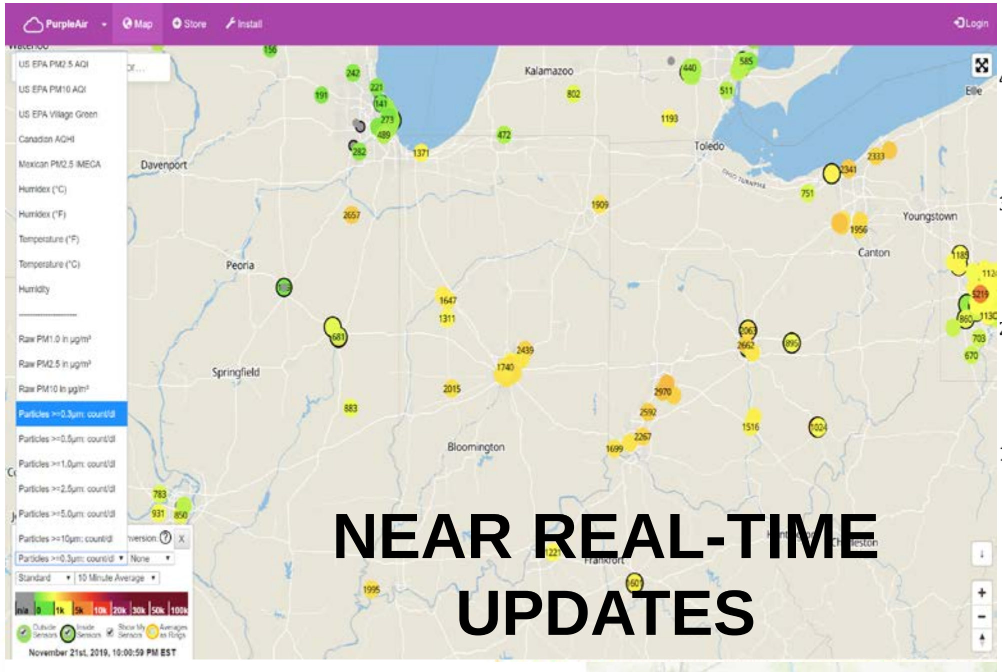




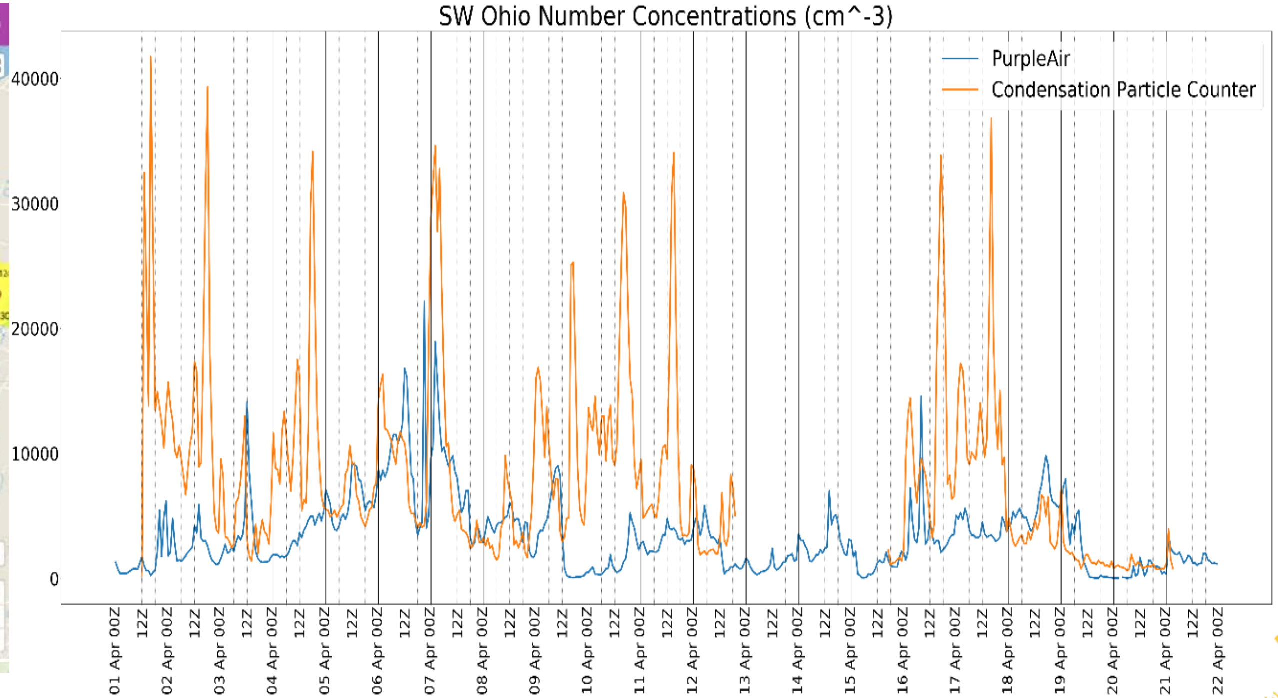
Hunter, 2007

PM$_{2.5}$ Observation

Organization	Standardized	Detection > 300-nm	Detection > 10-nm
Environmental Protection Agency (EPA)		✓	
Global Atmosphere Watch (GAW)	✓		✓
PurpleAir	✓	✓	

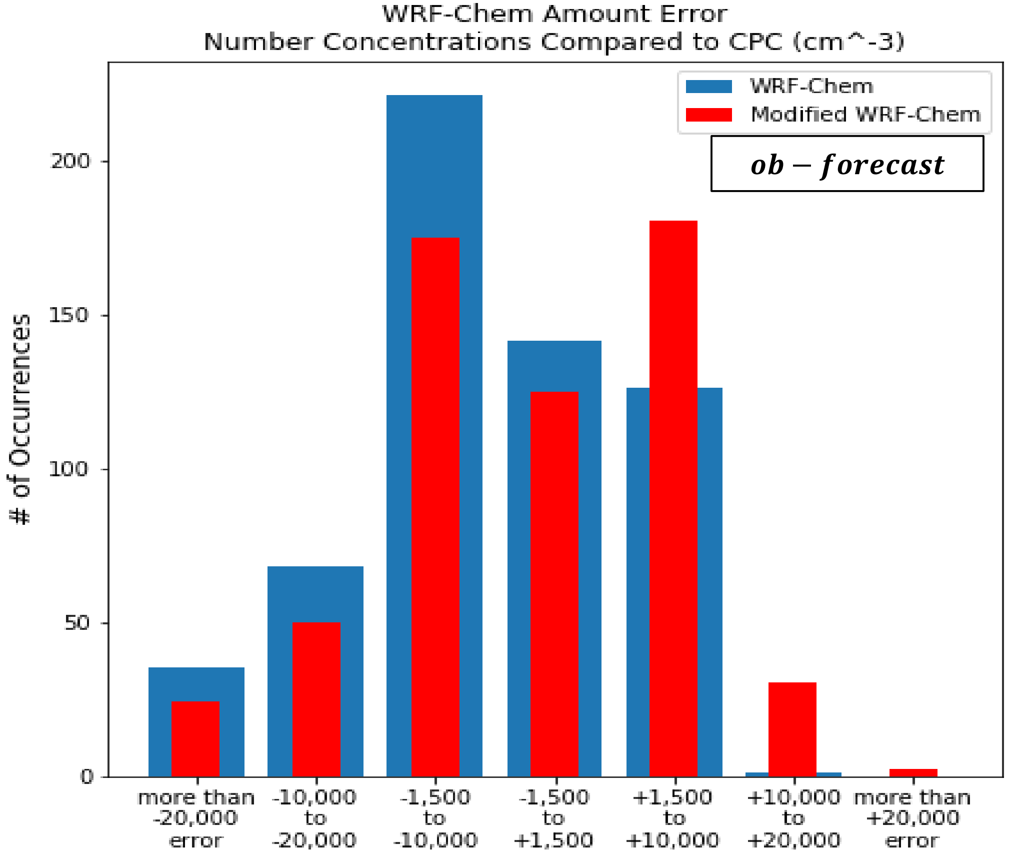


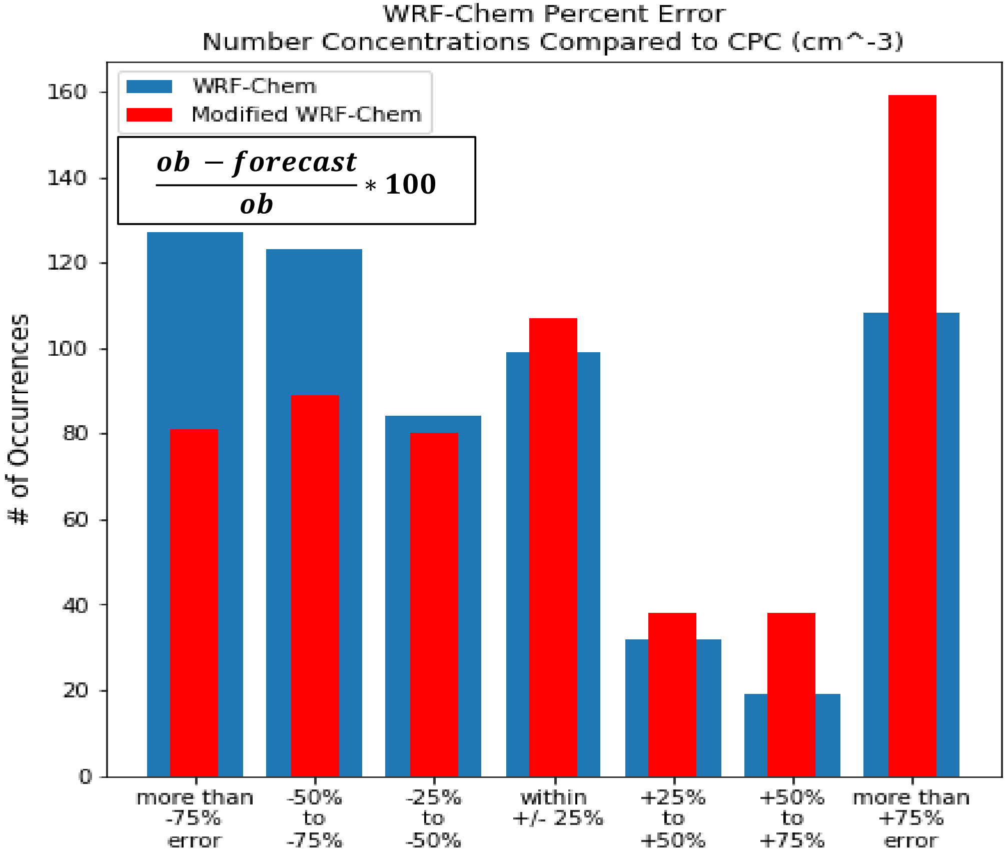
PurpleAir, 2020



Modified WRF-Chem

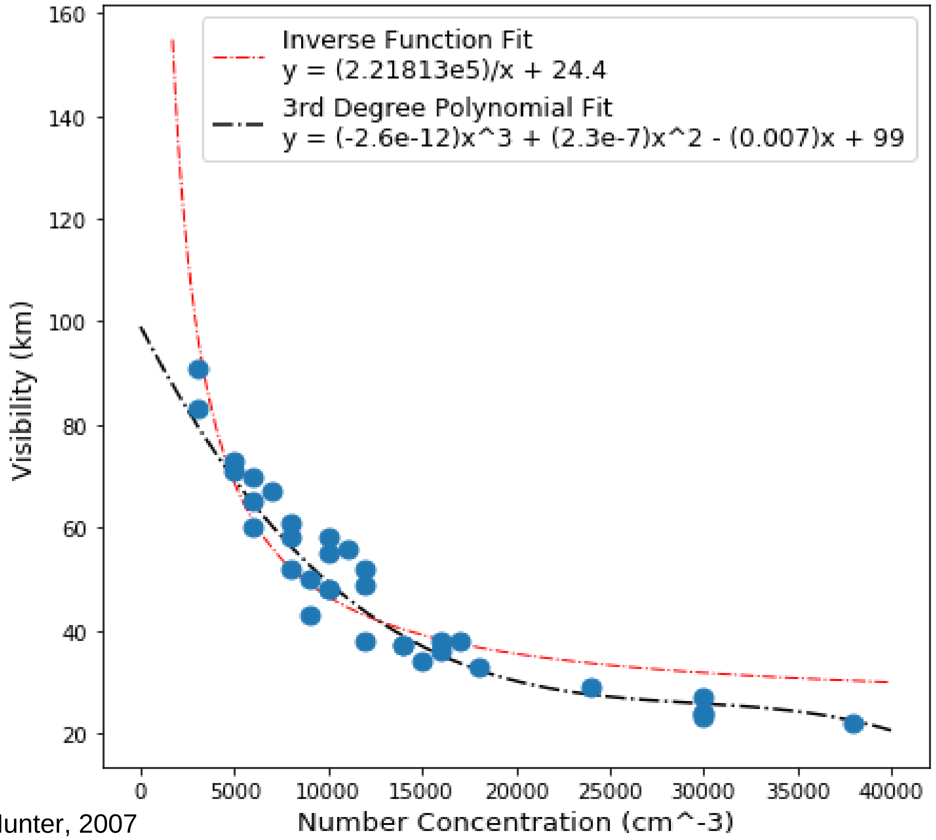
- Reduction in Underforecasts, Increase in Overforecasts
- Average Hourly Error – Reduced by 9%
  - within first 24hrs of forecast





Sustained Observation

- Horizontal Light Extinction
- Number → Visibility Conversion
- Fits Existing Ob Framework



Hunter, 2007

Number Concentration (cm⁻³)	Visibility (nearest ½ km or SM)	METAR VIS (Metric)	METAR VIS (Imperial)
Not Available	Transmissometer	VVVV	VV SM
0	99.0 // 60	9990	60 SM
2,500	82.5 // 51	9825	51 SM
5,000	69.0 // 43	9690	43 SM
7,500	58.0 // 36	9580	36 SM
10,000	49.0 // 31	9490	31 SM
12,500	42.0 // 26	9420	26 SM
15,000	36.5 // 23	9365	23 SM
17,500	32.5 // 20	9325	20 SM
20,000	30.0 // 19	9300	19 SM
22,500	28.0 // 18	9280	18 SM
25,000	27.0 // 17	9270	17 SM
27,500	26.0 // 16	9260	16 SM
30,000	25.5 // 16	9255	16 SM
32,500	25.0 // 15	9250	15 SM
35,000	24.0 // 15	9240	15 SM
37,500	22.5 // 14	9225	14 SM
40,000	20.5 // 13	9205	13 SM
42,500	17.0 // 11	9170	11 SM
45,000	12.5 // 8	9125	8 SM
47,500	6.5 // 4	9065	4 SM
50,000+	Transmissometer	VVVV	VV SM

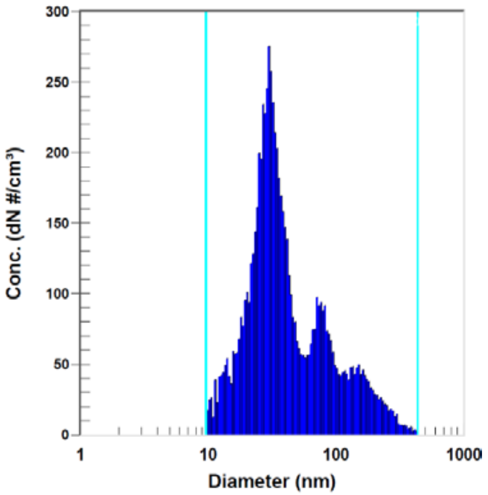
Research Objectives

1. Relevancy of $PM_{2.5}$ Number	✓	Captures Nano-Particle Abundance
2. Identify a Reliable Data Source	✓	PurpleAir is $0 but Needs Conversion
3. Improve WRF-Chem	✓	Reduction in Underforecasts
4. Introduce $PM_{2.5}$ to METAR	✓	Useful Data in a Familiar Format

Equations

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

N_d = *total particle density per unit volume* (normalized to 1)
r = *radius* (m)
r_M = *median radius* (m)
σ = *standard deviation*



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

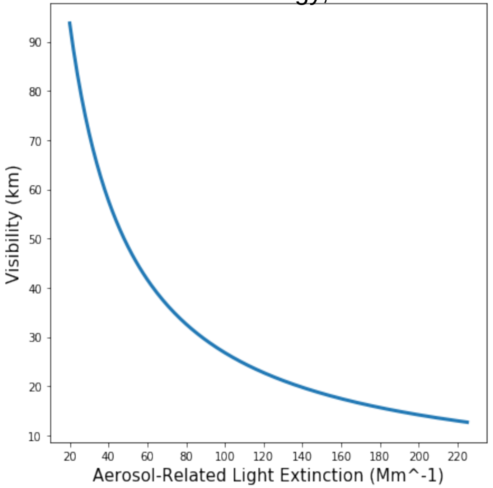
$Q_{e,s,a}(n,\lambda,r)$ = aerosol-constituent specific extinction, scattering, absorption

LEEDR
Laser Environmental Effects Definition And Reference

Center for Directed Energy, 2018

$$Surface\ Vis_{0.55\mu m} = \frac{3.0}{\beta_{e,a}(0)+\beta_{e,m}(0)} = \frac{3.0}{\beta_{e,a}(0)+0.012}$$

Visual contrast at 5% for human perception = 3.0-km
Average molecular extinction = 0.012-km^{-1}



Objective #4

Already noted that GOCART does not consider water-soluble aerosols

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)

- 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

Schmidt, 2019

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

AMERICAN METEOROLOGICAL SOCIETY

100th Annual Meeting 12 - 16 January 2020

AMS 100
ADVANCING SCIENCE
SERVING SOCIETY

Air Force Institute of Technology
Center for Directed Energy
Wright-Patterson AFB, Ohio

Assessment of Improved WRF-Chem $PM_{2.5}$ Characterization via Implementation of an Aerosol Measurement Network

D. B. Jagoda[1], S. T. Fiorino[1], S. E. Peckham[2], K. J. Keefer[1], and J. E. Schmidt[1]
AFIT Department of Engineering Physics & USACE Cold Region Research and Environmental Lab

Daniel.Jagoda@afit.edu Jaclyn.Schmidt.ctr@afit.edu Kevin.Keefer.ctr@afit.edu Steven.E.Peckham.civ@mail.mil Steven.Fiorino@afit.edu

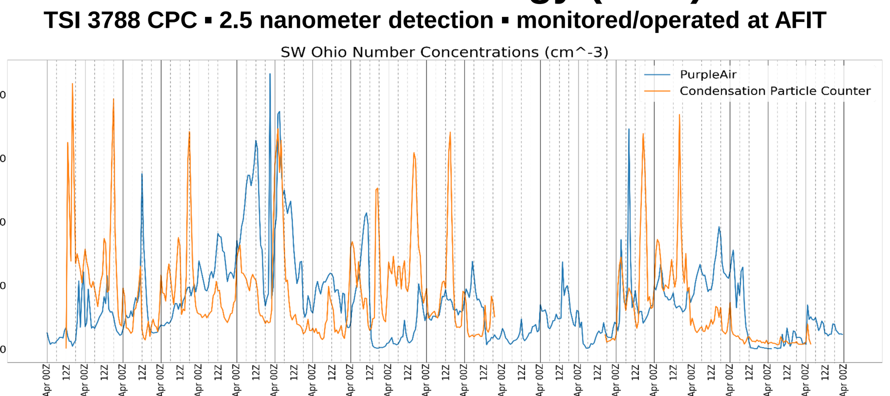
Atmospheric-chemistry NWP models use aerosol schemes based on climatic data instead of real-time observations. An advocation to monitor aerosol number concentration with a global sensor network is defended. A comparison between observations from the existing network "PurpleAir" and condensation particle counters (CPC) reveals the necessity of regulated instrumentation when measuring aerosol number concentration. Emission initialization of the Goddard Chemistry Aerosol Radiation and Transport (GOCART) scheme is capable of augmentation by hourly aerosol observation. The disparity between observed *in-situ* particulate matter smaller than 2.5-μm in diameter ($PM_{2.5}$) and Weather Research and Forecasting with Chemistry (WRF-Chem) output—with GOCART optioned—can be reduced via this augmentation. Analysis is done on WRF-Chem output near Dayton, Ohio after CPC data is utilized to modify GOCART input. Upon confirmation of improved WRF-Chem $PM_{2.5}$ characterization by point-observation initialization, a method of integrating an observational network is suggested: METAR encoding of $PM_{2.5}$ number concentration as a genuine horizontal visibility.

Research Objectives

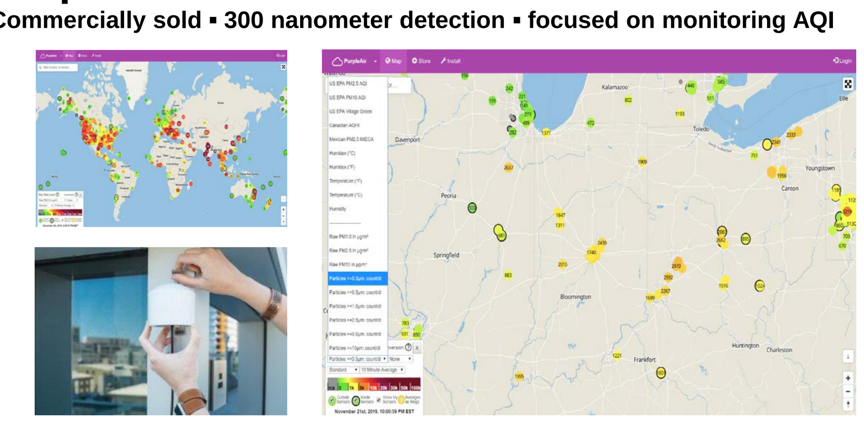
1. **Establish relevancy of atmospheric composition—particularly $PM_{2.5}$—to operational meteorology**
2. **Expose non-standardization within the aerosol measurement community**
3. **Advocate for real-time observation as a replacement for climatic data in NWP**
4. **Improve accuracy of WRF-Chem $PM_{2.5}$ characterization using augmentation by real-time data**
5. **Develop a method to introduce aerosol measurement to METAR reporting**

Aerosol Measurement
Methodologies and Scope from Four Organizations

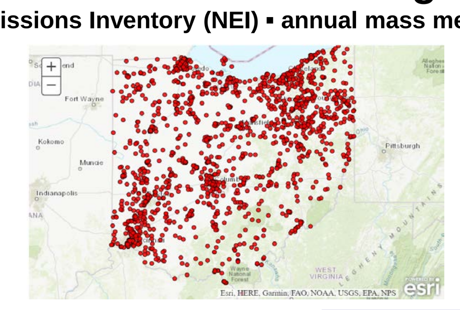
Center for Directed Energy (CDE)
TSI 3788 CPC • 2.5 nanometer detection • monitored/operated at AFIT



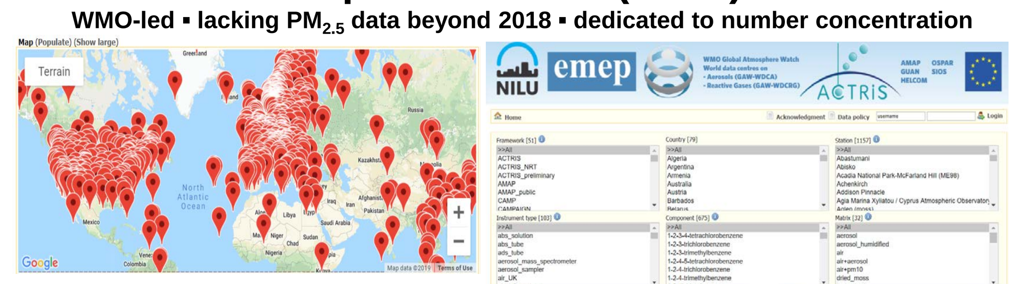
PurpleAir
Commercially sold • 300 nanometer detection • focused on monitoring AQI



Environmental Protection Agency (EPA)
National Emissions Inventory (NEI) • annual mass measurements



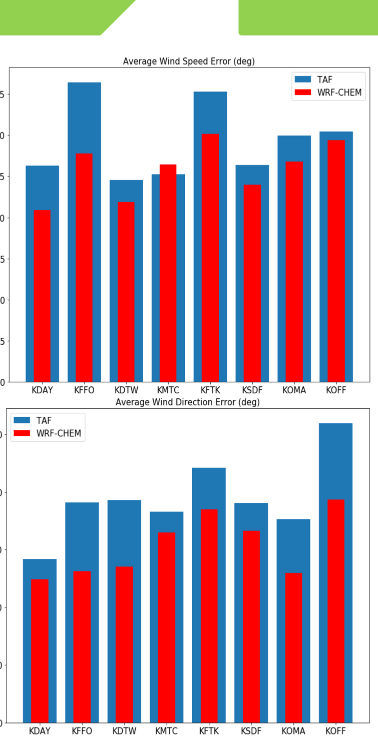
Global Atmosphere Watch (GAW)
WMO-led • lacking $PM_{2.5}$ data beyond 2018 • dedicated to number concentration



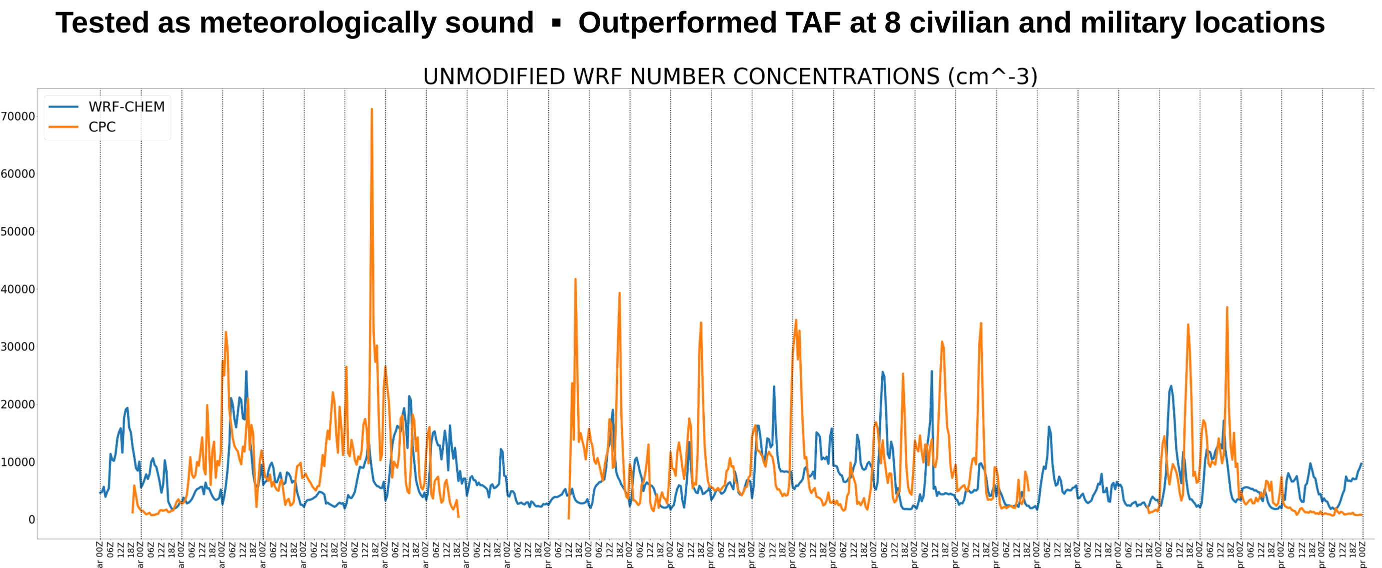
Comparing WRF-Chem Output
Pre/Post Input Manipulation

WPS GFS and Gridded Data → **Real** Initialization → **Chem** GOCART w/ EDGAR-HTAP → **Input Modification** → **ARW** WRF v3.8 → **Output** netCDF format

Before Augmentation



Tested as meteorologically sound ▪ Outperformed TAF at 8 civilian and military locations



Average 6222 particles/cm^3 error ▪ Average 125% disparity from measured

After Augmentation

Meteorologically unaffected

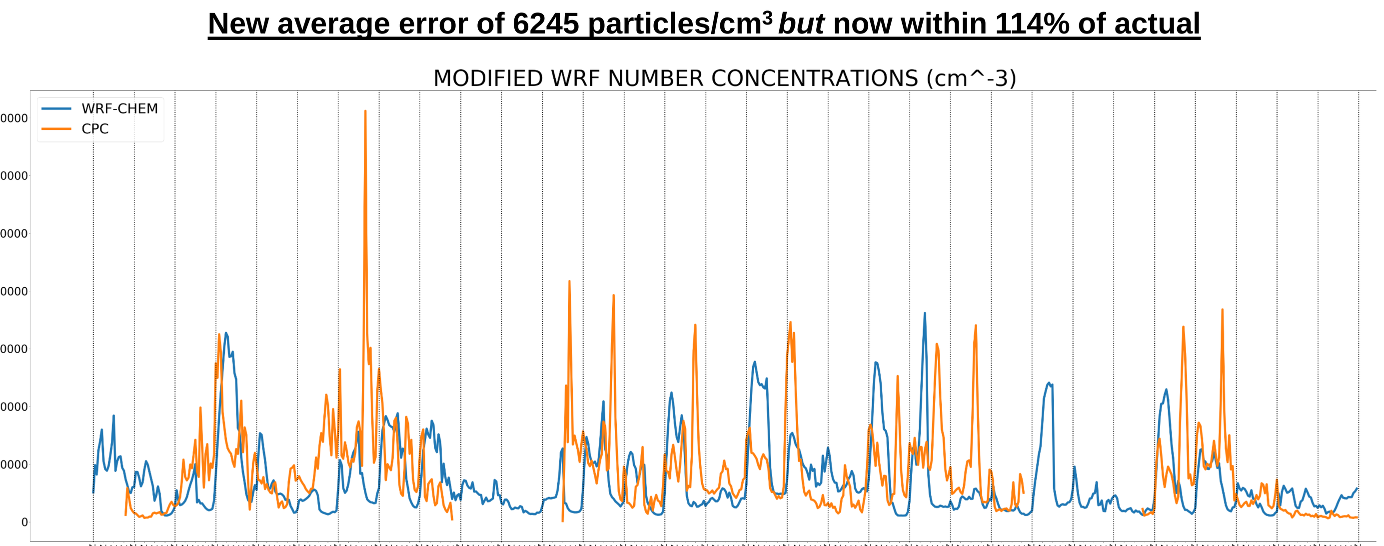
Daytime Median Radius set to 75-nm 12Z-02Z in Ohio

Nighttime Median Radius set to 90-nm 02Z-11Z

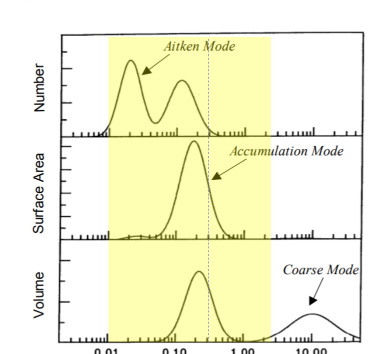
WRF-Chem peaks nearer magnitude of CPC

Largest increases within first 12 hours of each model run

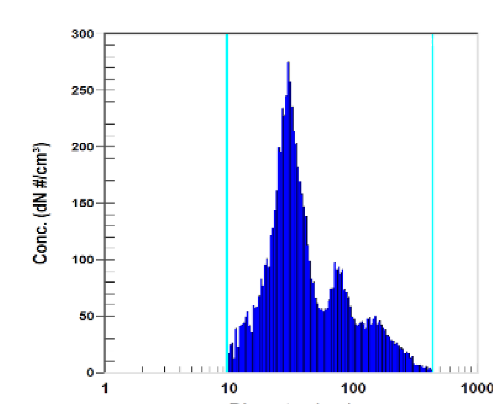
New average error of 6245 particles/cm^3 *but* now within 114% of actual



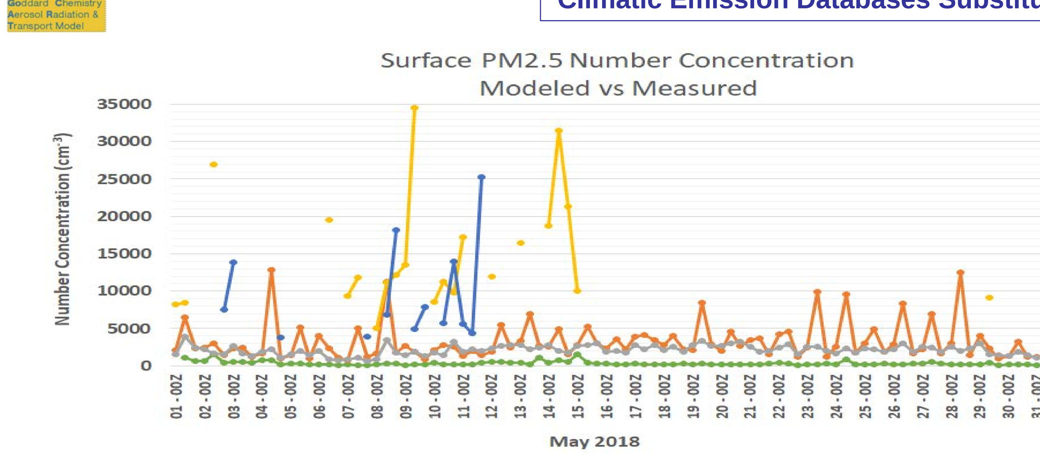
$PM_{2.5}$ – Number vs Mass

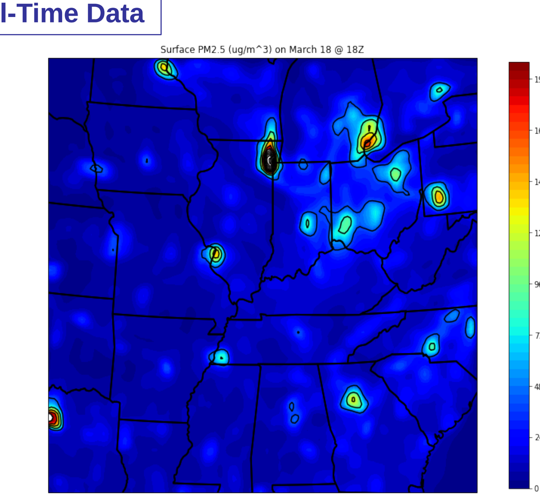


- **Mass measurement favors particles in coarse mode**
- **Fine particles linked to:**
  cloud formation
  backscattering
  health degradation
- **Number measurement with lognormal size distribution encompasses both Aitken and accumulation modes**



NWP Aerosol Schemes
Climatic Emission Databases Substitute for Real-Time Data





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

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

$$dM_i = dN_i * m_i$$

$$dM_i = dN_i * \rho_i V_i$$

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

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

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

Grafting a Network into Operations
Visibility Categories in METAR Format

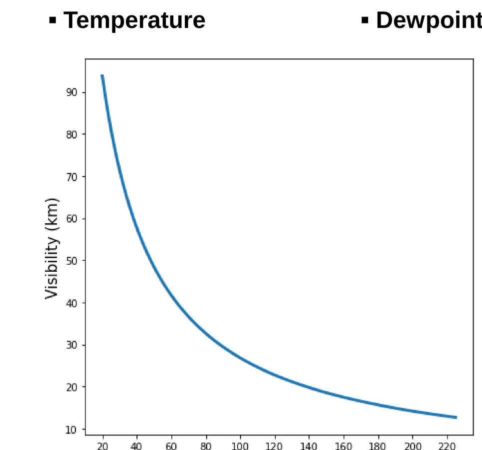
Current METAR format loses value when visibility is >10 SM or 9999

Report VIS via conversion from number concentration

Number Concentration (cm^{-3})	Visibility (nearest ½ km or SM)	METAR VIS (Metric)	METAR VIS (Imperial)
Not Available	Transmissometer	XXXX	XX SM
0	99.0 // 60	9990	60 SM
2,500	82.5 // 51	9825	51 SM
5,000	69.0 // 43	9690	43 SM
7,500	58.0 // 36	9580	36 SM
10,000	49.0 // 31	9490	31 SM
12,500	42.0 // 26	9420	26 SM
15,000	36.5 // 23	9365	23 SM
17,500	32.5 // 20	9325	20 SM
20,000	30.0 // 19	9300	19 SM
22,500	28.0 // 18	9280	18 SM
25,000	27.0 // 17	9270	17 SM
27,500	26.0 // 16	9260	16 SM
30,000	25.5 // 16	9255	16 SM
32,500	25.0 // 15	9250	15 SM
35,000	24.0 // 15	9240	15 SM
37,500	22.5 // 14	9225	14 SM
40,000	20.5 // 13	9205	13 SM
42,500	17.0 // 11	9170	11 SM
45,000	12.5 // 8	9125	8 SM
47,500	6.5 // 4	9065	4 SM
50,000+	Transmissometer	XXXX	XX SM

LEEDR calculates $\beta_{e,a}$ using 4 inputs at desired λ and *n*

- **Number Concentration**
- **Temperature**
- **Pressure**
- **Dewpoint**



Number-Size Distribution (lognormal)

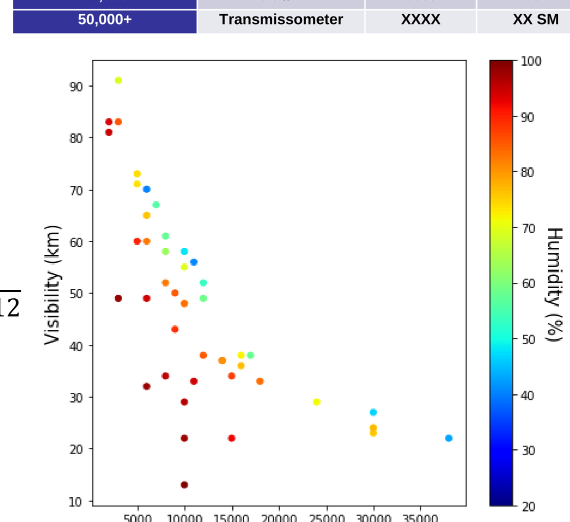
$$[1] \quad \frac{dN(r)}{d(\log r)} = \frac{N}{(2\pi)^{1/2}\log(\sigma)}\exp\left[-\frac{(\log r - \log r_M)^2}{2(\log\sigma)^2}\right]$$

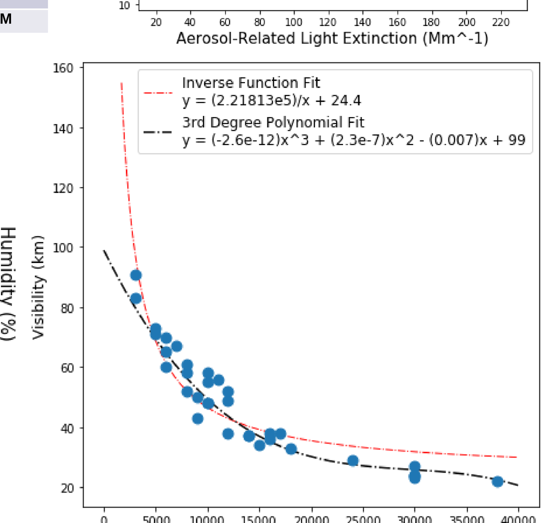
The Mie Extinction

$$[2] \quad \beta_{e,s,a}(\lambda) = \int_{r_1}^{r_2} Q_{e,s,a}(n,\lambda,r)\pi r^2 \frac{dN(r)}{r\ln 10 d(\log r)}dr \approx \sum_{i=r_{min}}^{r_{max}} Q_{e,s,a}(n,\lambda,r_i)\pi r_i^2 \frac{dN_i}{r_i \ln 10 d(\log r_i)}\Delta r_i$$

Converting to a Usable Visibility

$$[3] \quad Surface\ Vis_{0.55\mu} = \frac{3.0}{\beta_{e,a}(0) + \beta_{e,m}(0)} = \frac{3.0}{\beta_{e,a}(0) + 0.012}$$





Future Research

- **Test WRF-Chem in other regions, during other seasons, and during longer time periods**
- **Deploy CPCs at various locations or use PurpleAir sensors as input for WRF-Chem**
- **Generate more test points for visibility comparison between LEEDR and a transmissometer**
- **Generate discussion amongst aerosol-observation organizations to standardize measurements**

A special thanks to the DoD Directed Energy Joint Technology Office and CRREL ERDC for funding support

[1]Air Force Institute of Technology
[2]Cold Regions Research and Engineering Laboratory (CRREL) Engineer Research and Development Center (ERDC)

The views expressed in this document are those of the author(s) and do not reflect the official policy or position of the United States Air Force, the Department of Defense, or the United States government.