



Theoretical Basis for Converting Satellite Observations to Ground-Level $PM_{2.5}$ Concentrations

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NASA Air Quality Remote Sensing Training, US EPA, Raleigh, NC, March 20-23, 2023

Objectives



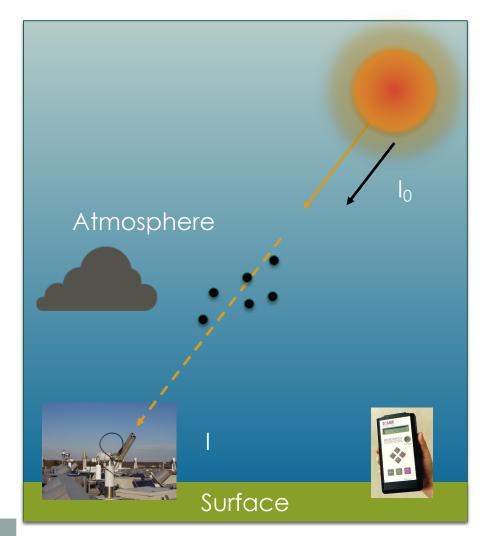
By the end of this presentation, you will have an understanding of:

• Methods to estimate $PM_{2.5}$ mass concentration at surface level (µg m⁻³) while using satellite derived Aerosol Optical Depth (AOD) at visible wavelengths



Optical Depth





The optical depth expresses the quantity of light removed from a beam by **scattering** and/or **absorption** during its path through a medium.

Optical Depth τ as:

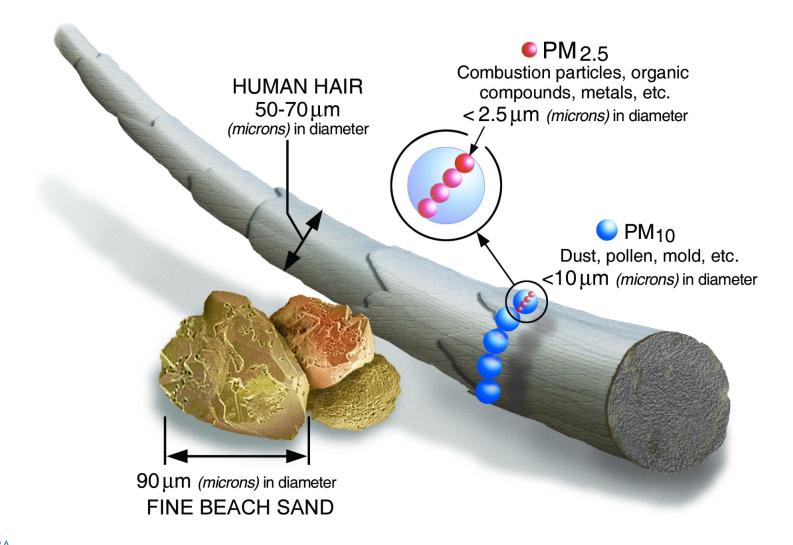
$$I = I_o e^{-m\tau}$$

$$m = \sec \theta_0$$

$$\tau = \tau_{Rayl} + \tau_{aer} + \tau_{gas}$$



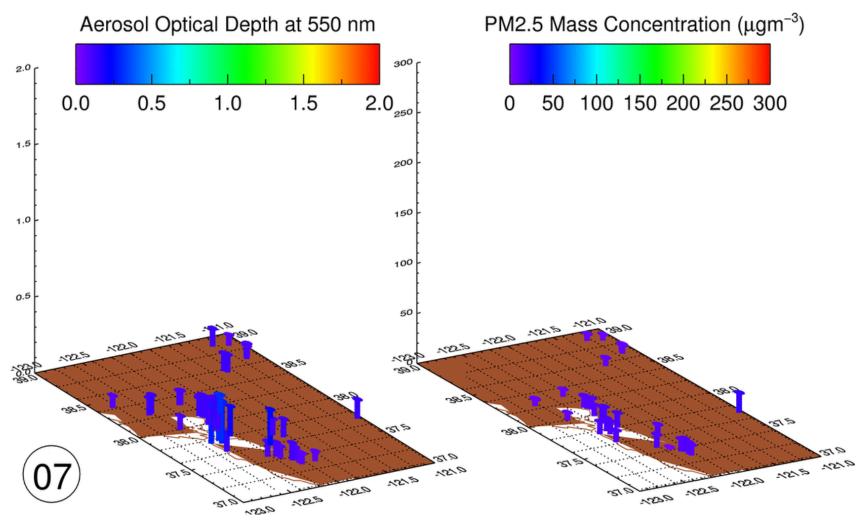
PM_{2.5}





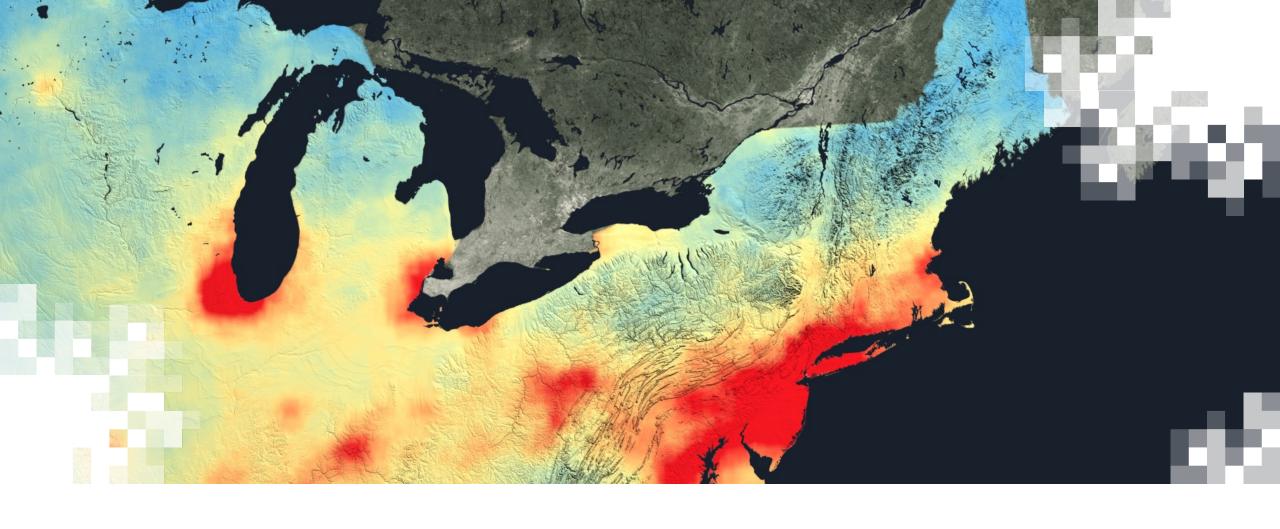


Surface vs. Satellite Measurements





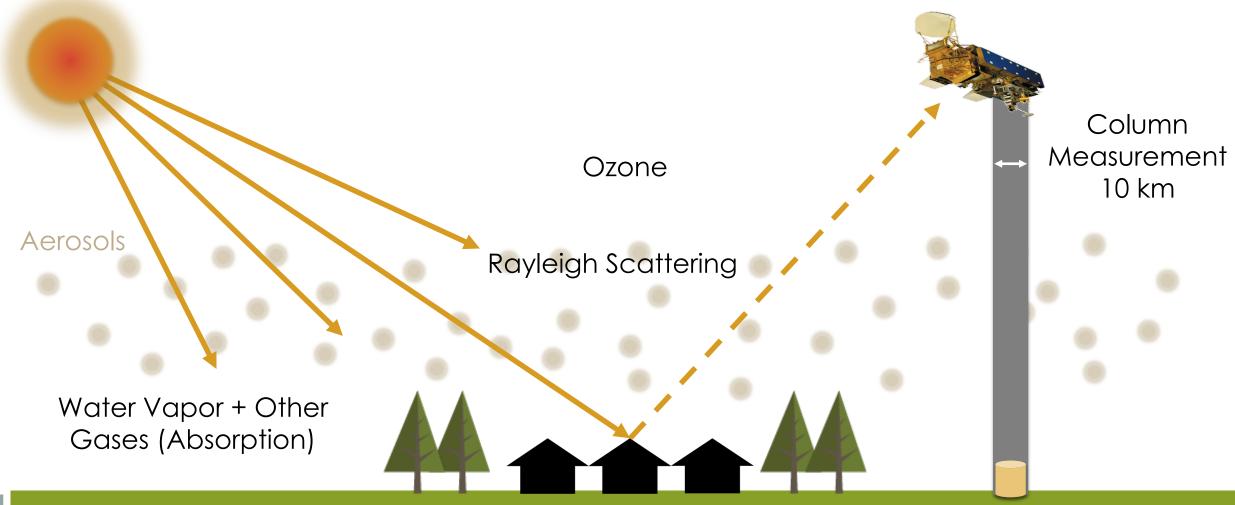




AOD (or AOT) to PM

Aerosol Optical Depth from Satellites



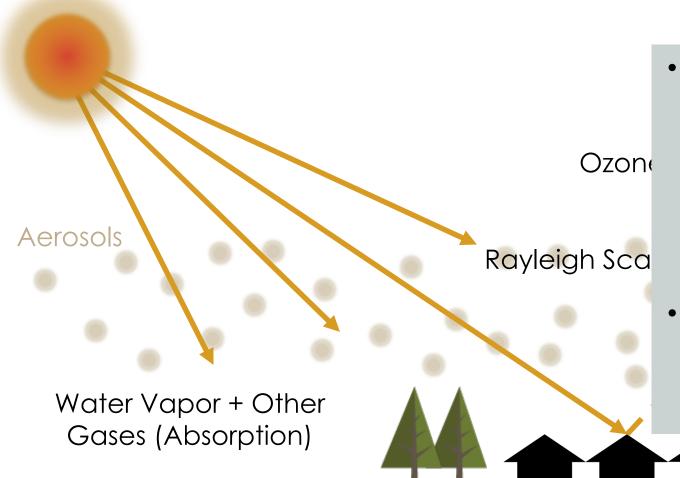






Aerosol Optical Depth from Satellites





- AOT(τ)= $\int \beta_{ext} dz$
 - Particle Size
 - Composition
 - Water Update
 - Vertical Distribution
- There are satellite retrieval issues.
 - Inversion (e.g., aerosol model, background)

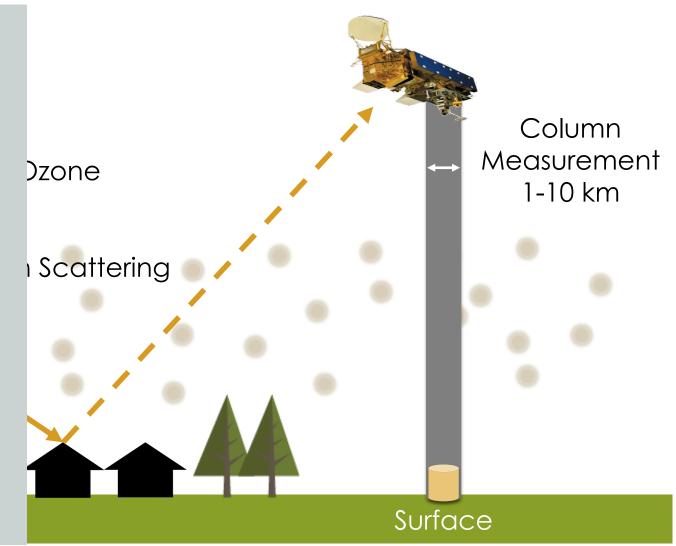




Aerosol Optical Depth from Satellites

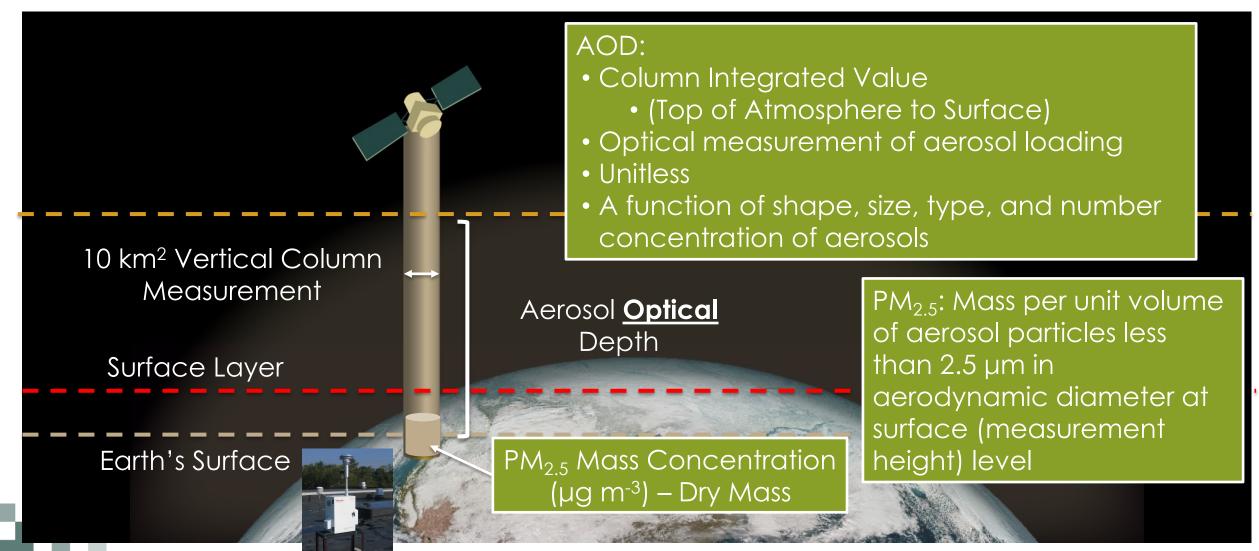
m

- Seven MODIS bands are utilized to derive aerosol properties.
 - $0.47 \mu m$
 - $-0.55 \, \mu m$
 - $-0.65 \mu m$
 - $-0.86 \, \mu m$
 - $-1.24 \, \mu m$
 - $-1.64 \, \mu m$
 - $2.13 \mu m$
- 10x10 km² resolution
- 6x6 km² resolution
- 3x3 km² resolution
- 1x1 km² resolution
- 0.75x0.75 km² resolution



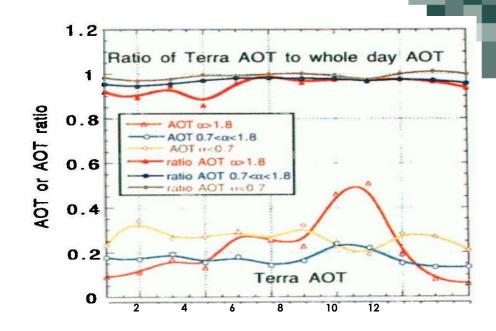


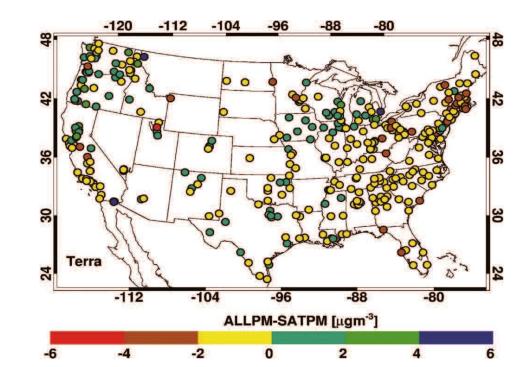
Satellite vs. Ground Observation

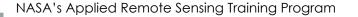


Support for AOD-PM_{2.5} Linkage

- Satellite AOD is sensitive to $PM_{2.5}$.
 - Kahn et al. 1998
- Polar-orbing satellites can represent at least daytime average aerosol loadings.
 - Kaufman et al. 2000
- Missing data due to cloud cover appear random in general.
 - Gupta and Christopher, 2008
 - Christopher and Gupta, 2010







AOD-PM Relationship



Assuming cloud-free skies, a well mixed boundary layer with no overhead aerosols, and aerosols that have similar optical properties*, AOD and $PM_{2.5}$ can be related by this equation:

$$\tau = PM_{2.5} \text{ H f}(RH) \frac{3Q_{ext,dry}}{4 \rho r_{eff}}$$

- т: AOD at 550 nm
- p: Aerosol Mass Density
- r_e: Particle Effective Radius
- Q: Extinction Coefficient

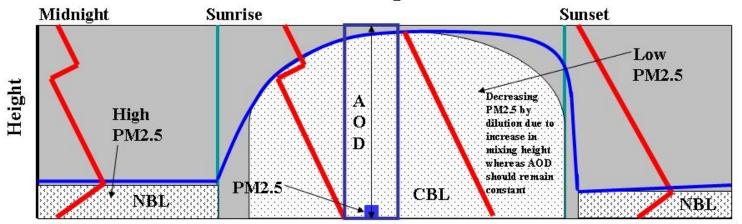
- H: Mixing Height
- f(RH): How aerosol scattering changes with changing relative humidity

Source: Hoff, R. & Christopher, S., 2009

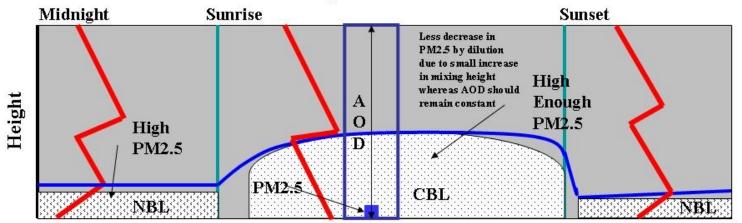


Vertical Mixing

Weak and High Inversion Case



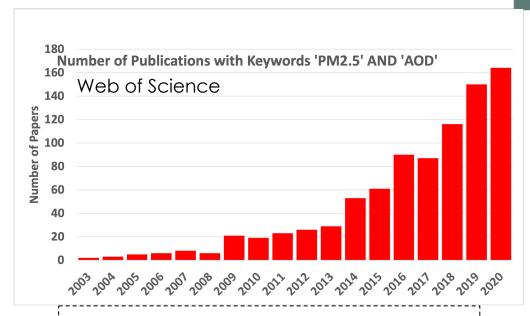
Strong and low Inversion Case





Particulate Matter (PM) from Satellites

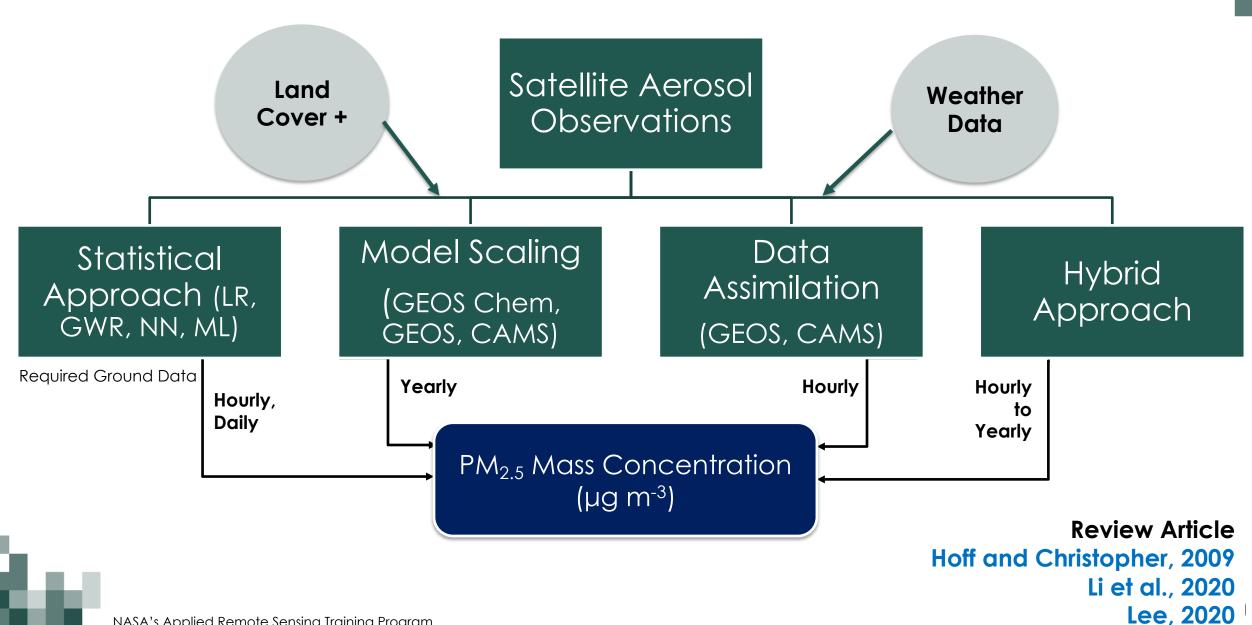
- Kaufman and Fraser, 1983, Fraser et al., 1984
 - AOD and Sulfate from GOES-VISSR
- Wang and Christopher, 2003, Chu et al., 2003
 - AOD & $PM_{2.5}$ (and PM_{10}) relationship
- Liu et al., 2004, van Donkelaar et al., 2006
 - Used CTM to scale AODs to $PM_{2.5}$
- Gupta and Christopher, 2009
 - Used Artificial Intelligence to convert AOD to PM_{2.5}
- van Donkelaar et al., 2010, 2015, 2019, 2021
 - Global Product Annual & Monthly Mean
- Shaddick et al., 2017, 2018
 - Bias corrected annual $PM_{2.5}$ data for WHO, SDGs
- Di et al., 2019 Daily CONUS PM_{2.5} (MAIAC)
- Hai and Kondragunta, 2021 Hourly/Daily from VIIRS & GOES-R



Research on AOD to $PM_{2.5}$ conversion is growing exponentially, but we only have annual & monthly mean global products and no daily or sub-daily operational global products from satellites.



Almost Two Decades of Research and Learning

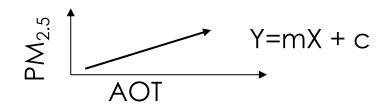


PM_{2.5} Estimation: Popular Methods





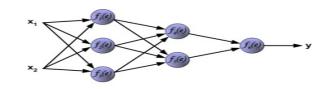
Two-Variable Method



Multivariable Method

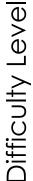
$$PM_{2.5} = \beta_0 + \alpha \times \tau + \sum_{n=1}^{\infty} (\beta_n x_{n-1}^{*} M_n)$$

Artificial Intelligence/ML/D



MSC

Model Surface Area Concentration x Satellite AOD Estimated $PM_{2.5} =$ Model AOD





PM_{2.5} Estimation: Two Variable Method (TVM)

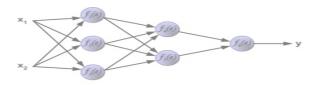


Two-Variable Method Y=mX+c AOT

Multivariable Method

$$PM_{2.5} = \beta_0 + \alpha \times T + \sum (\beta_n \underset{n=1}{\overset{m}{\times}} M_n)$$

Artificial Intelligence



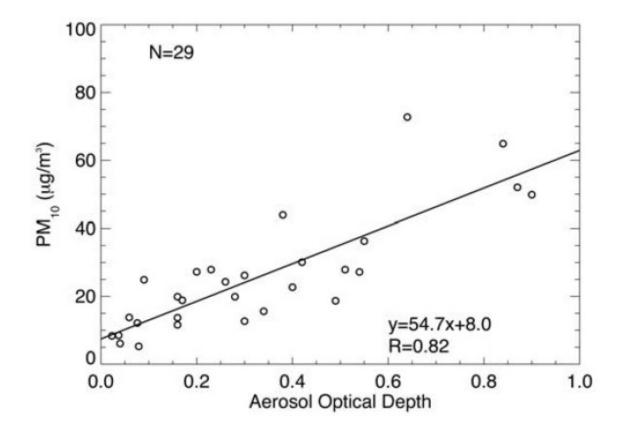
MSC

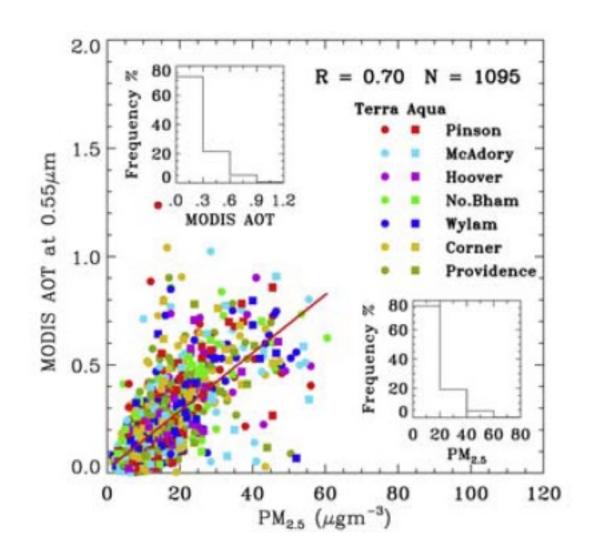
Estimated PM_{2.5} = Model Surface Area Concentration x Satellite AOD

Model AOD



Simple Models from Early Days

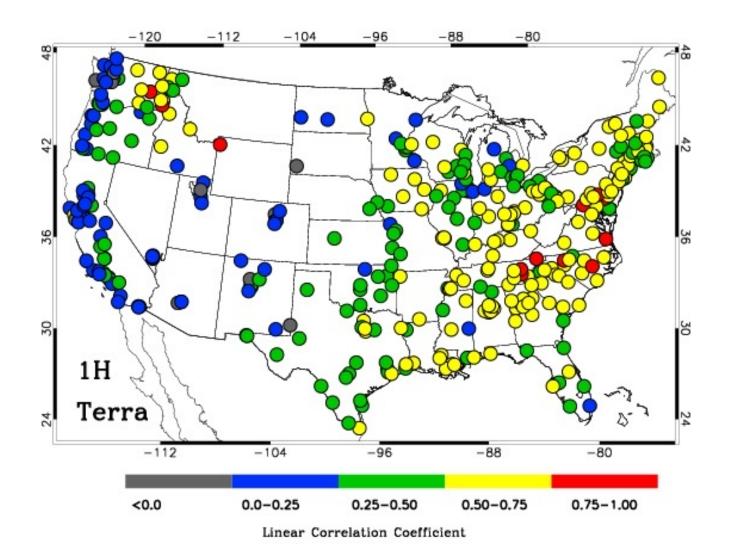


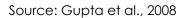


(Left) Chu et al., 2003; (Right) Wang et al., 2003



AOD-PM_{2.5} Relationship







PM_{2.5} Estimation: Multivariable Method (MVM)

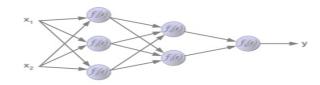


Two-Variable Method Y=mX+c AOT

Multivariable Method

$$PM_{2.5} = \beta_0 + \alpha \times \tau + \sum_{n=1}^{\infty} (\beta_n \times M_n)$$

Artificial Intelligence



MSC

Estimated PM_{2.5} = Model Surface Area Concentration x Satellite AOD

Model AOD

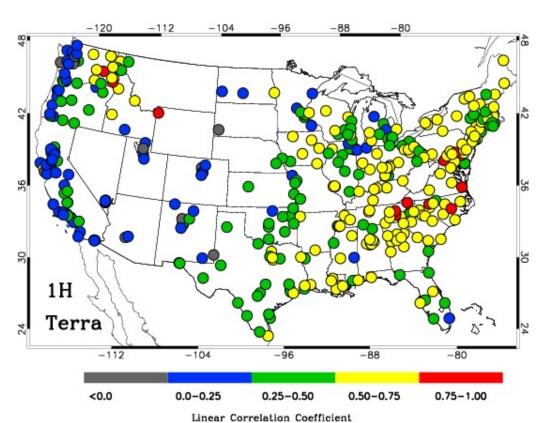
A A C



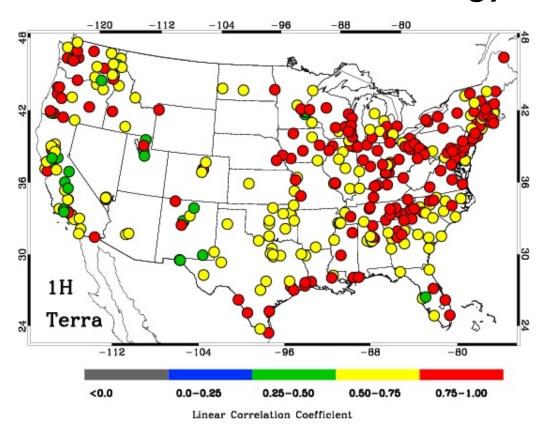
Multivariable Method (MVM)

en,

Predictor: AOD



Predictor: AOD + Meteorology



Linear Correlation Coefficient Between Observed and Estimated PM_{2.5}

Source: Gupta et al., 2008



Multivariable Method – Beyond Meteorology

en,

- Advanced Regression Analysis with More Input Parameters
 - Land Cover Type
 - Forest Cover, Shrub Cover
 - Urban %
 - DEM (Altitude)
 - Road Length
 - Population Density
 - Snow Fraction
 - Shortwave Radiation
 - NDVI

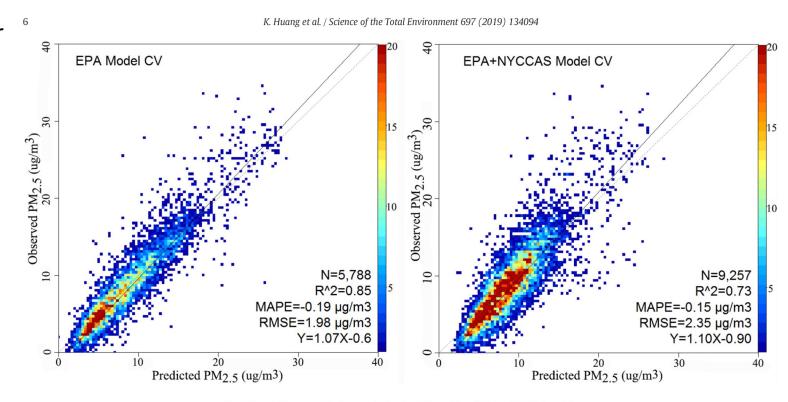


Fig. 2. Ten-fold cross-validation results for the EPA model and EPA + NYCCAS models.

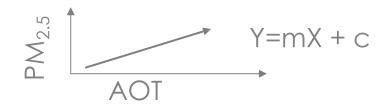
https://www.sciencedirect.com/science/article/pii/S0048969719340719



PM_{2.5} Estimation: Artificial Intelligence (or ANN)

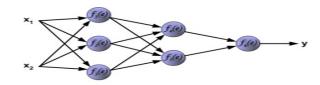


Two-Variable Method



$$PM_{2.5} = \beta_0 + \alpha \times T + \sum_{n=1}^{\infty} (\beta_n \times M_n)$$

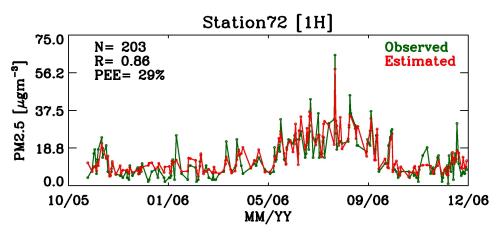
Artificial Intelligence

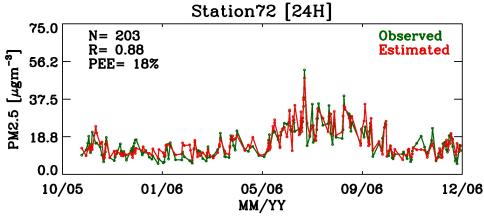


Model Surface Area Concentration x Satellite AOD Estimated $PM_{2.5} =$ Model AOD

Examples of Results from ANN & RF







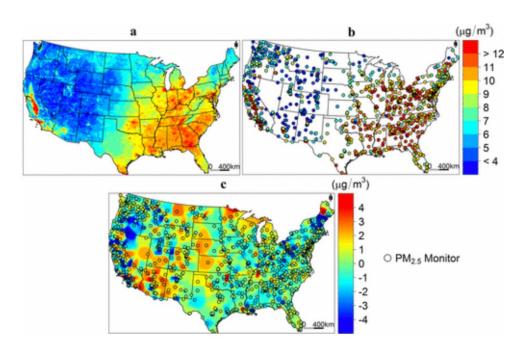


Figure 4. Annual mean predictions. (a) Annual mean $PM_{2.5}$ predictions over the continental United States for 2011; (b) annual mean $PM_{2.5}$ measurements at ground monitors; (c) difference between annual mean predictions and observations at ground monitors and difference interpolations over the continental United States.

Source: Gupta 2009, Hu et al., 2017



PM_{2.5} Estimation: Model Scaling (MSC)

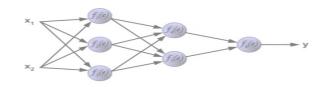


Two-Variable Method Y=mX+c AOT

Multivariable Method

$$PM_{2.5} = \beta_0 + \alpha \times T + \sum_{n=1}^{\infty} (\beta_n \times M_n)$$

Artificial Intelligence



MSC

Estimated PM_{2.5} = Model Surface Area Concentration x Satellite AOD Model AOD



Scaling Approach



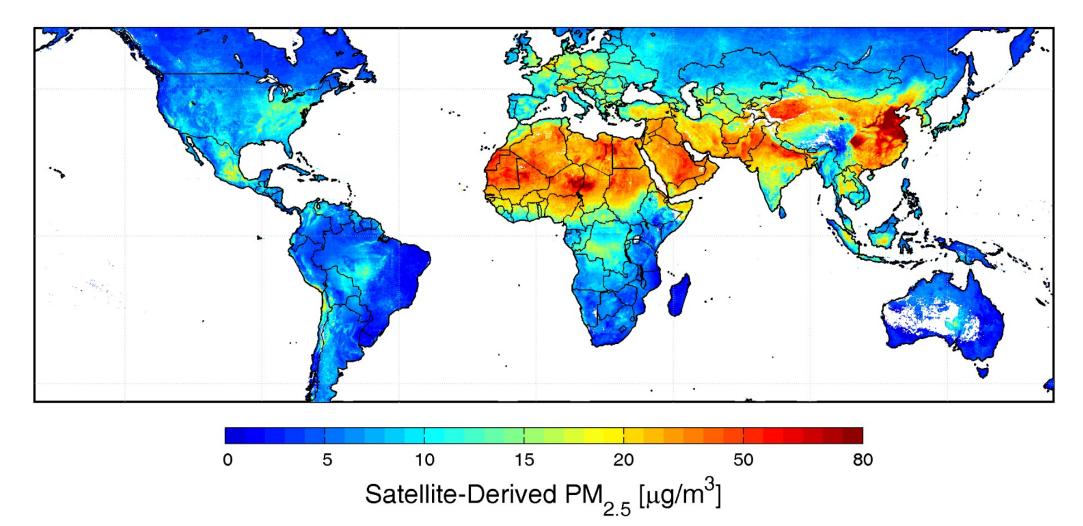
- Basic Idea:
 - Let an atmospheric chemistry model decide the conversion from AOD to $PM_{2.5}$.
 - Satellite AOD is used to calibrate the absolute value of the model-generated conversion ratio.

• Satellite-Derived
$$PM_{2.5} = \left(\frac{PM_{2.5}}{AOD}\right) \times Satellite AOD$$





Annual Mean PM_{2.5} from Satellite Observations



Source: von Donkelaar et al., 2006, 2009



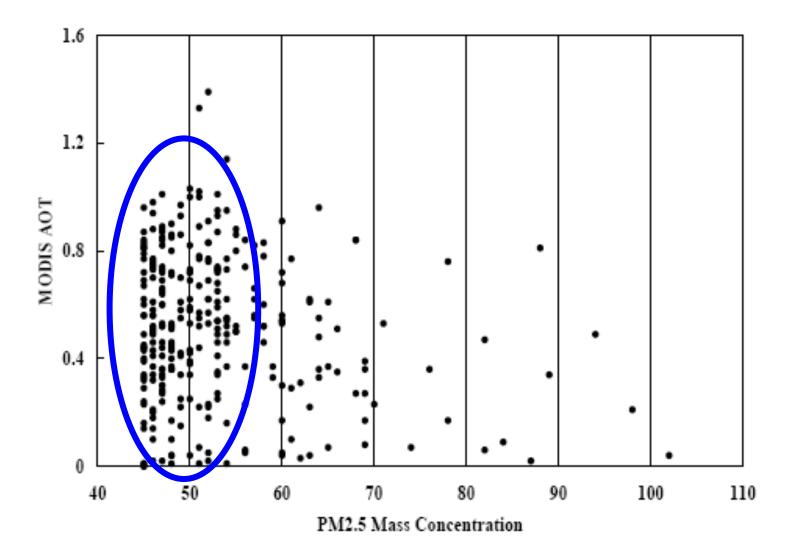
Questions to Ask: Issues



- How accurate are these estimates?
- Is the PM_{2.5} AOD relationship always linear?
- How does AOD retrieval uncertainty impact estimation of air quality?
- Does this relationship change in space and time?
- Does this relationship change with aerosol type?
- How does meteorology drive this relationship?
- How does the vertical distribution of aerosols in the atmosphere impact these estimates?



Limitation: Vertical Distribution of Aerosols

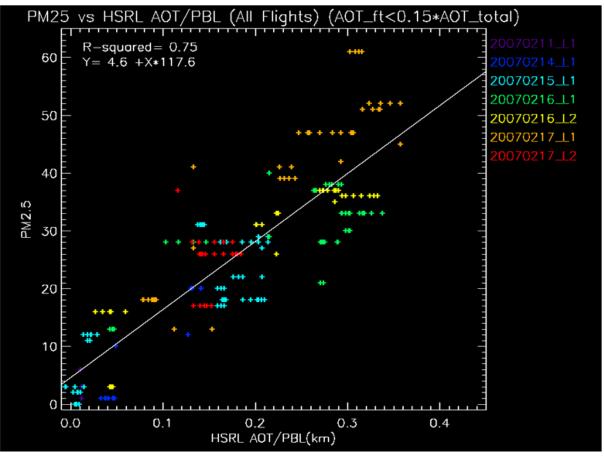






Vertical Distribution: Impact on AOD-PM_{2.5}

- Normalizing AOD with boundary layer height significantly improves the correlation with surface $PM_{2.5}$ (R² increases from 0.36 to 0.75).
- With accurate estimates of PBL height, AOD can be a good proxy for $PM_{2.5}$.



Source: Al-Saadi et al., 2008



Assumption for Quantitative Analysis



When most particles are concentrated and well mixed in the boundary layer, satellite AOD contains a strong signal of ground-level particle concentrations.

No Textbook Solution



Use of Satellite Data



- Currently for Research & Applications
 - Spatial distribution of $PM_{2.5}$ on a regional to national level
 - Long term trends of $PM_{2.5}$
 - Model calibration, data assimilation, and validation
 - Exposure assessments for health effect studies
 - Spatial trends at urban scales
 - Improved coverage and accuracy
 - Fused statistical-deterministic models
- For Regulation?



Suggested Reading

http://www.nsstc.uah.edu/sundar/papers/2009/AWMA-proof.pdf

2009 CRITICAL REVIEW

ISSN:1047-3289 J. Atr & Waste Manage. Assoc. 59:645-675 DOI:10.3155/1047-3289.59.6.645 Copyright 2009 Air & Waste Management Association





Raymond M. Hoff

Remote Sensing of Particulate Pollution from Space: Have We Reached the Promised Land?

Department of Physics and the Joint Center for Earth Syst and Technology Center, University of Maryland, Baltimore (

Sundar A. Christopher

Alabama-Huntsville, Huntsville, AL

IMPLICATIONS

Satellite measurements are going to be an integral part of the Global Earth Observing System of Systems. Satellite measurements by themselves have a role in air quality Department of Atmospheric Sciences and Earth System Sciences but cannot stand alone as an observing system. Data assimilation of satellite and ground-based measurements into forecast models has synergy that aids all of these air quality tools.

> the "but for" provision in the rule makes the use of satellite data possible in significant exceedances only. Applications such as event identification, transport, and atmospheric composition determination are strengths of satellite measurements. Where high precision is required (compliance monitoring, the "but for" test, and quantitative measurement of visibility effects on Class I areas), satellite data are presently of limited utility.

The use of the AOD as a measure for mass concentration has skill in some regions but less in others and does not provide a uniform way to measure aerosols across the United States. We discussed in Table 4 the range of mea-

In 2007, the A&WMA Critical Review by Bachmann discussed the history of the National Ambient Air Quality Standards (NAAQS). 142 The 39-yr history of those standards parallels the time period that satellite meteorology and observations have developed and yet, to date, no satellite measurements have been used to quantitatively address the NAAQS. From the review conducted here, only one congres-

EPA has taken a satellite observations role for itself in the Exceptional Events Rule.144 If a region can show conclusively that they are being impacted by an event (a fire, a dust storm, etc.) that is outside of their jurisdiction to regulate, the event can be flagged as a nonexceedance event. This provides a significant motivation for regional

Although the desire for the use of satellite data for air quality purposes is widely stated, the reality is that many of the measurements have not yet met the promise that they can be operationally used for today's air quality monitoring requirements. Precision in measuring AOD is



More Review Articles





A Review on Predicting Ground PM_{2.5} Concentration Using Satellite Aerosol Optical Depth

Yuanyuan Chu 1,2,†, Yisi Liu 1,†, Xiangyu Li 1,2, Zhiyong Liu 3, Hanson Lu 4, Yuanan Lu 2,5, Zongfu Mao 1,2, Xi Chen 1, Na Li 1, Meng Ren 1, Feifei Liu 1, Liqiao Tian 6, Zhongmin Zhu 6,7 and Hao Xiang 1,2,*

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- 3 The National Environmental Satellite, Data, and Information Service (NESDIS), National Oceanic and Atmospheric Administration (NOAA), 5830 University Research Court, College Park, MD 20740, USA; Zhiyonglau@gmail.com
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- State Key Laboratory of Information Engineering in Surveying, Mapping and Remote Sensing, Wuhan University, 129# Luoyu Road, Wuhan 430079, China; tianligiao@whu.edu.cn (L.T.); zhongmin.zhu@whu.edu.cn (Z.Z.)
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- Correspondence: xianghao@whu.edu.cn; Tel.: +86-27-6875-9118
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Remote Sensing of Environment 269 (2022) 112827



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Remote Sensing of Environment





Review

A review of statistical methods used for developing large-scale and long-term PM2.5 models from satellite data

Zongwei Ma^{a,*}, Sagnik Dey^{b,c}, Sundar Christopher^d, Riyang Liu^a, Jun Bi^a, Palak Balyan^b, Yang Liu e,

- State Key Laboratory of Pollution Control and Resource Reuse, School of the Environment, Nanjing University, Nanjing, Jiangsu, China Centre for Atmospheric Sciences, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India
- Centre of Excellence for Research on Clean Air, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, India d Department of Atmospheric and Earth Science, University of Alabama in Huntsville, USA
- Gangarosa Department of Environmental Health, Rollins School of Public Health, Emory University, Atlanta, GA, USA

ARTICLE INFO

Editor: Menghua Wang

Keywords-Satellite remote sensing Aerosol optical depth PM_{2.5} estimates Statistical methods

ABSTRACT

Research of PM2.5 chronic health effects requires knowledge of large-scale and long-term exposure that is no supported by newly established monitoring networks due to their sparse spatial coverage and lack of historica measurements. Estimating PM_{2.5} using satellite-derived aerosol optical depth (AOD) can be used to fill the data gap left by the ground monitors and extend the PM2.5 data coverage to suburban and rural areas over long time periods. Two approaches have been applied in large-scale and long-term satellite remote sensing of PM2.5, i.e., the scaling and statistical approaches. Compared to the scaling method, the statistical approach has greater prediction accuracy and has been widely used. There is a gap in the current literature and review papers on how the statistical methods work and specific considerations to best utilize them, especially for large-scale and longterm estimates. In this critical review, we summarize the evolution of large-scale and long-term PM2 = statistical models reported in the literature. We describe the framework and guidance of large-scale and long-term satellite based PM2.5 modeling in data preparation, model development, validation, and predictions. Sample computer codes are provided to expedite new model-building efforts. We also include useful considerations

https://www.scie ncedirect.com/s cience/article/pi i/S003442572100 5472

https://www.researchaate.n et/profile/Hyung-Joo-Lee/publication/348104773 **Advancing Exposure Assess** ment of PM25 Using Satellit e Remote Sensing A Revie w/links/60bc5ad6458515218 f94cec3/Advancing-**Exposure-Assessment-of-**PM25-Using-Satellite-Remote-Sensing-A-Re

Review Article

Advancing Exposure Assessment of PM_{2.5} Using Satellite Remote Sensing: A Review

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Received: 31 August 2020 Revised: 28 October 2020 Accepted: 28 October 2020

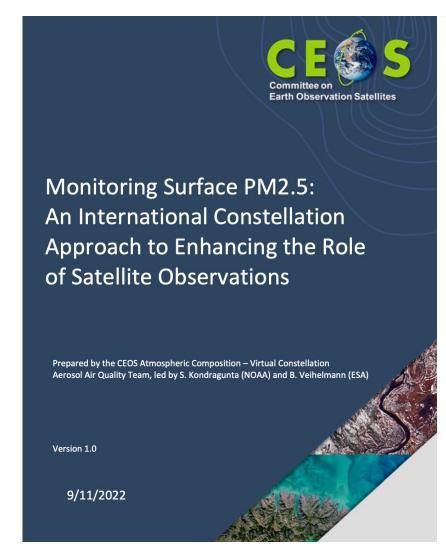
ABSTRACT Epidemiological studies have reported the associations of adverse health outcomes with ambient particulate matter with aerodynamic diameter $\leq 2.5 \,\mu m \, (PM_{2.5})$. While these studies have accumulated increasingly refined evidence on PM_{2.5}-health associations, the needs for more advanced PM_{2.5} exposure models have also grown. For the last two decades, PM_{2.5} estimation approaches using satellite remote sensing have been developed and advanced, taking advantage of quantitative aerosol data (e.g., aerosol optical depth; AOD), the development of satellite instruments and data retrieval algorithms, and the application of statistical and machine learning techniques. Subsequently, the satellite-based PM_{2.5} concentrations have contributed to health effect studies by providing spatially resolved exposure estimates of ambient PM25 and thus reducing exposure misclassification. This article summarizes previous development and recent advancement of satellite-based PM_{2.5} exposure assessment in the context of satellite aerosol products and PM_{2.5} estimation methodologies. Furthermore, this article deals with enhanced satellite capabilities of generating the exposure estimates of PM_{2.5} composition and time-resolved PM2.5. Finally, the future directions of satellite-based exposure assessment are discussed based on research needs and the satellite remote sensing technology of addressing them.

KEY WORDS AOD, Environmental epidemiology, Exposure assessment, PM25, Public health, Satellite remote sensing



Remote Sensing of PM2.5 – White Paper

https://ceos.org/document_management/Meetings/SIT-Technical-Workshop/2022-SIT-Tech-Workshop/Documents/CEOS%20AC-VC%20White%20Paper%20PM2.5%20Monitoring%20Draft-version-4.1%2026-7-2022.pdf



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Dubovik, Oleg (LOA)

Fougnie, Bertrand (EUMETSAT)

Garrigues, Sébastien (ECMWF)

Giles, David (NASA)

Goldberg, Mitch (NOAA)

Gupta, Pawan (NASA/USRA)

Hashimoto, Makiko (JAXA) Henderson, Barron (EPA)

Holben, Brent (NASA)

Huff, Amy (IM Systems Group)

Kahn, Ralph (NASA)

Kim, Jhoon (Yonsei University)

Knowland, K. Emma (NASA/Morgan State University)

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Laszlo, Istvan (NOAA)

Lefer, Barry (NASA)

Levy, Rob (NASA)

Liu, Hongqing (IM Systems Group)

Liu, Yang (Emory University)

Loyola, Diego (DLR)

Lyapustin, Alexei (NASA)

Martin, Randall (Washington University)

Mishra, Manoj (ISRO)

Muva, Ramana (ISRO)

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Tanaka, Taichu (JMA)

Torres, Omar (NASA)

van Donkelaar, Aaron (Dalhousie University)

Wang, Jun (U of Iowa)

Welton, Judd (NASA)

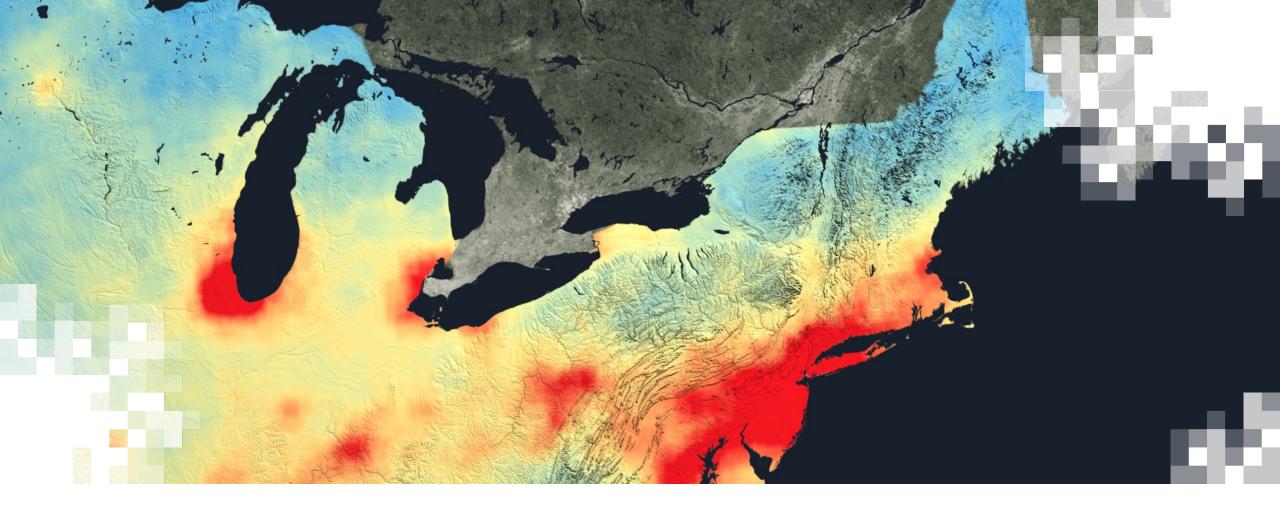
Zhang, Hai (IM Systems Group)



Suggested References

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Questions?