# Source Estimation Using Inversions


*Presenter:* Chris Loughner

*Other Team Members:* Tianfeng Chai, Hyun-Cheol Kim, Alice Crawford, Allison Ring

NOAA Air Resources Laboratory


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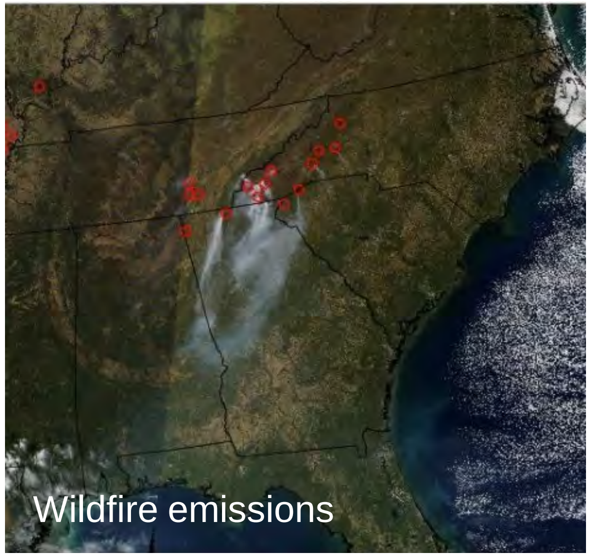
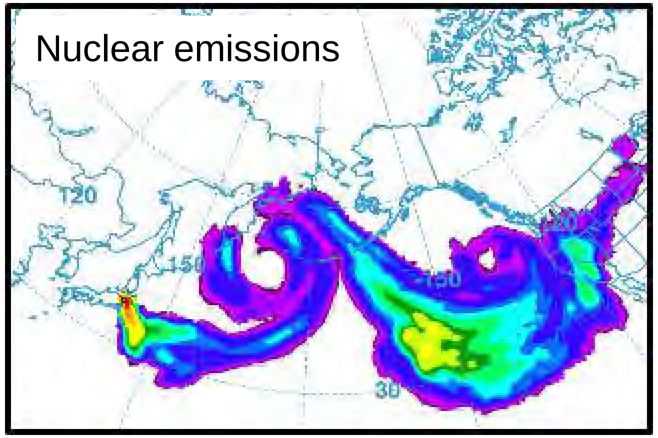
# Source Estimation Using Inversions

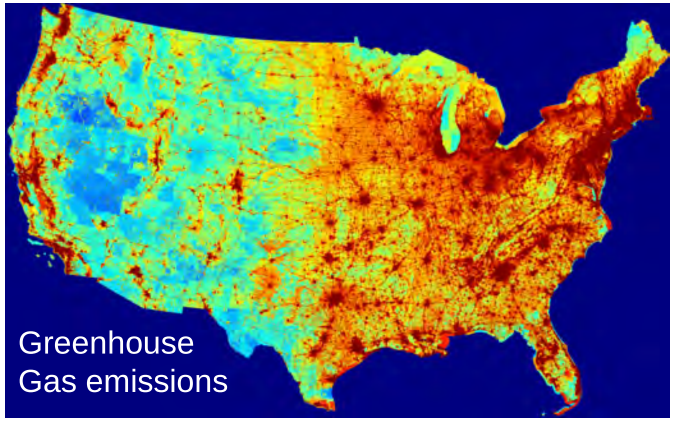
Volcanic emissions



Wildfire emissions



Nuclear emissions



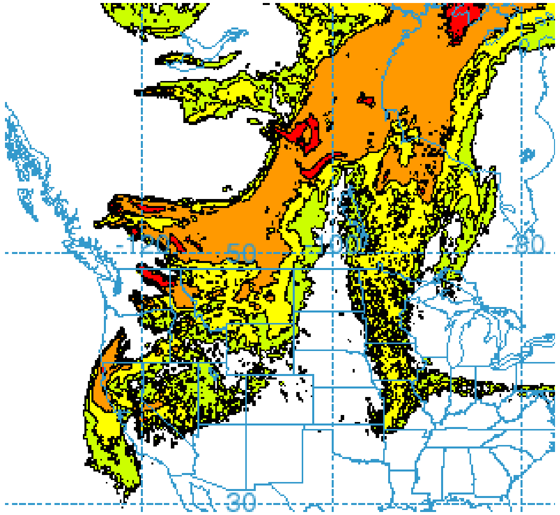
Greenhouse Gas emissions

- Improve emissions estimates, which are then used to make forecasts better.
- Improve greenhouse gas flux estimates to aid in meeting greenhouse gas emissions reductions targets.
- Improve nuclear, wildfire, volcanic, chemical, and greenhouse gas emissions.

# Relevance to OAR Strategic Goals

## Make forecasts better

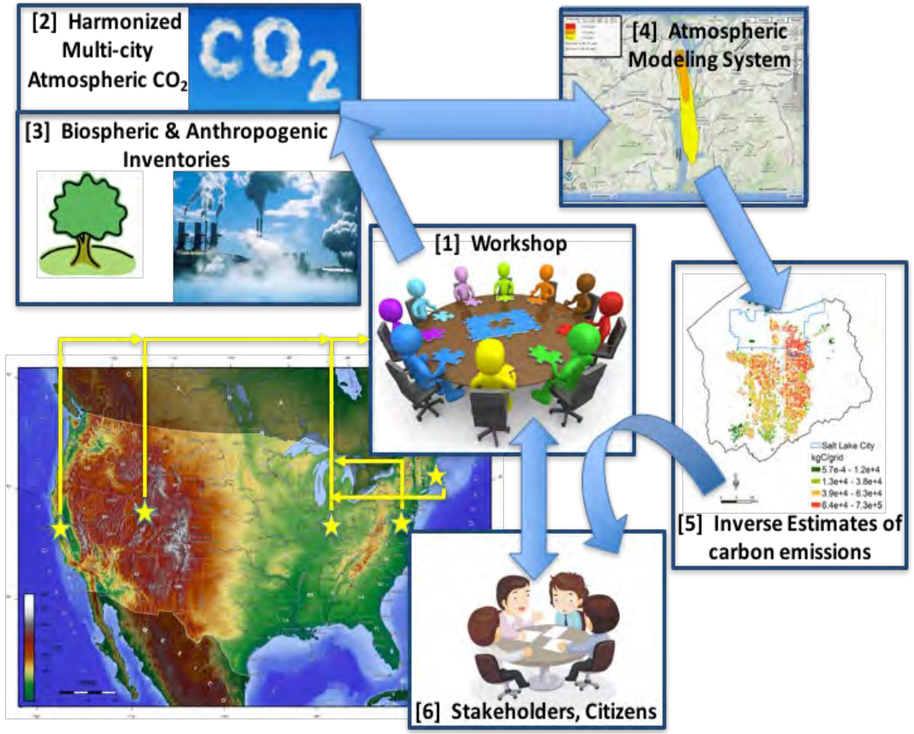
Improve accuracy, precision, and efficiency of forecasts and predictions to save lives and property and support a vibrant economy.



## Detect changes in the atmosphere

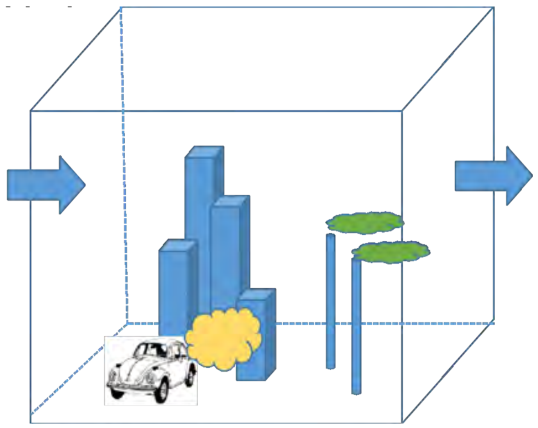
Produce, analyze, and interpret observation records to understand the Earth system and inform the public.

Evaluate greenhouse gas emissions inventories, assess if greenhouse gas emissions reduction targets are on track, and identify sources for emissions reductions strategies.



# Source Estimation Using Inversions

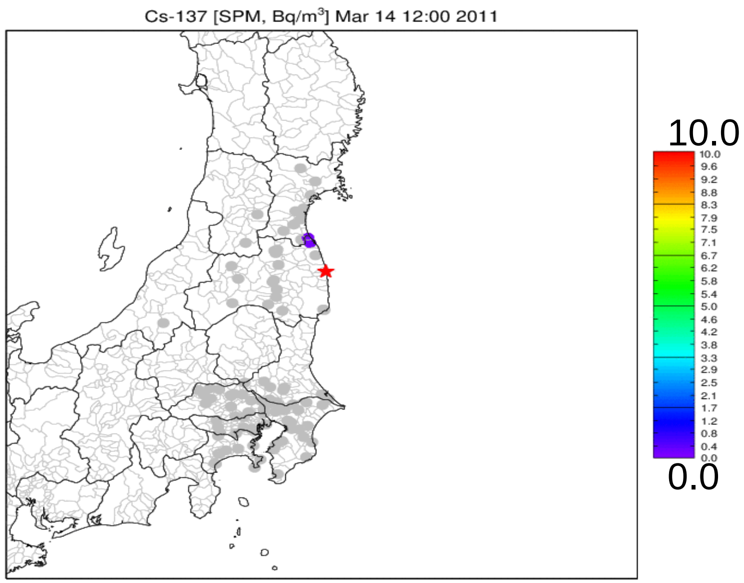
**Types of inversions**



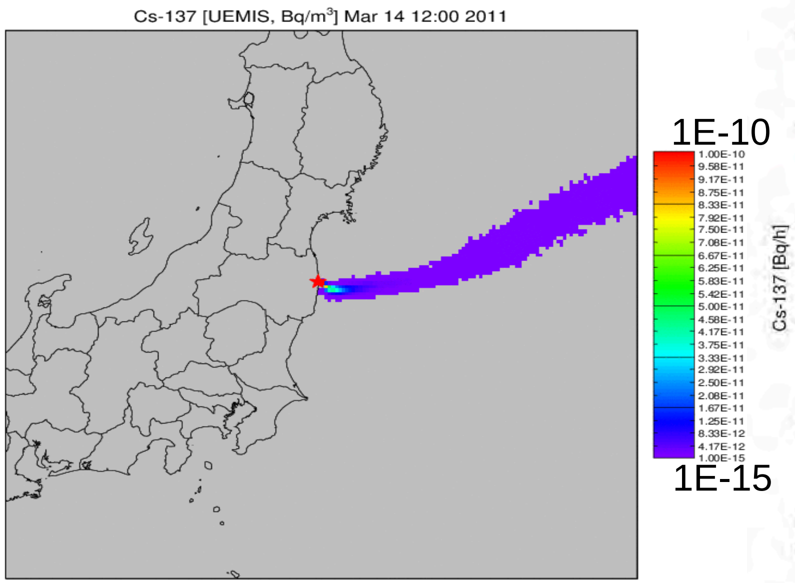
- Mass balance approach:
  - Observe concentrations upwind and downwind of source region to estimate emissions
- Transfer Coefficient Matrix – Cost Function approach
  - HYSPLIT run with unit emissions for multiple possible realizations (location and time) to generate a Transfer Coefficient Matrix (TCM)
  - Source terms are solved by minimizing a cost function to measure the differences between model predictions and observations
- Bayesian inversion
  - Optimize emissions estimates by minimizing a cost function that includes:
    - *prior emissions estimates* (typically from a bottom-up inventory)
    - *background concentration estimates*
    - *model footprints* = locations where surface fluxes can influence observation; obtained from backward HYSPLIT dispersion simulations from observational location
    - *error covariance matrices* - represent the uncertainty in prior fluxes and measurement-model mismatch

# Fukushima source term estimation

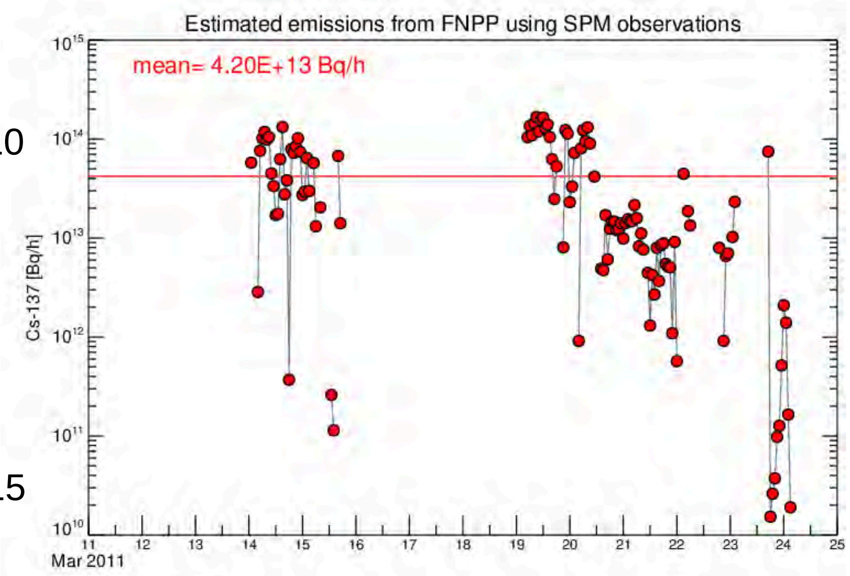
TCM approach used to estimate Fukushima source term using Japanese domestic observations of Cs-137.




Cs-137 concentrations Bq/m$^3$
(SPM monitors)



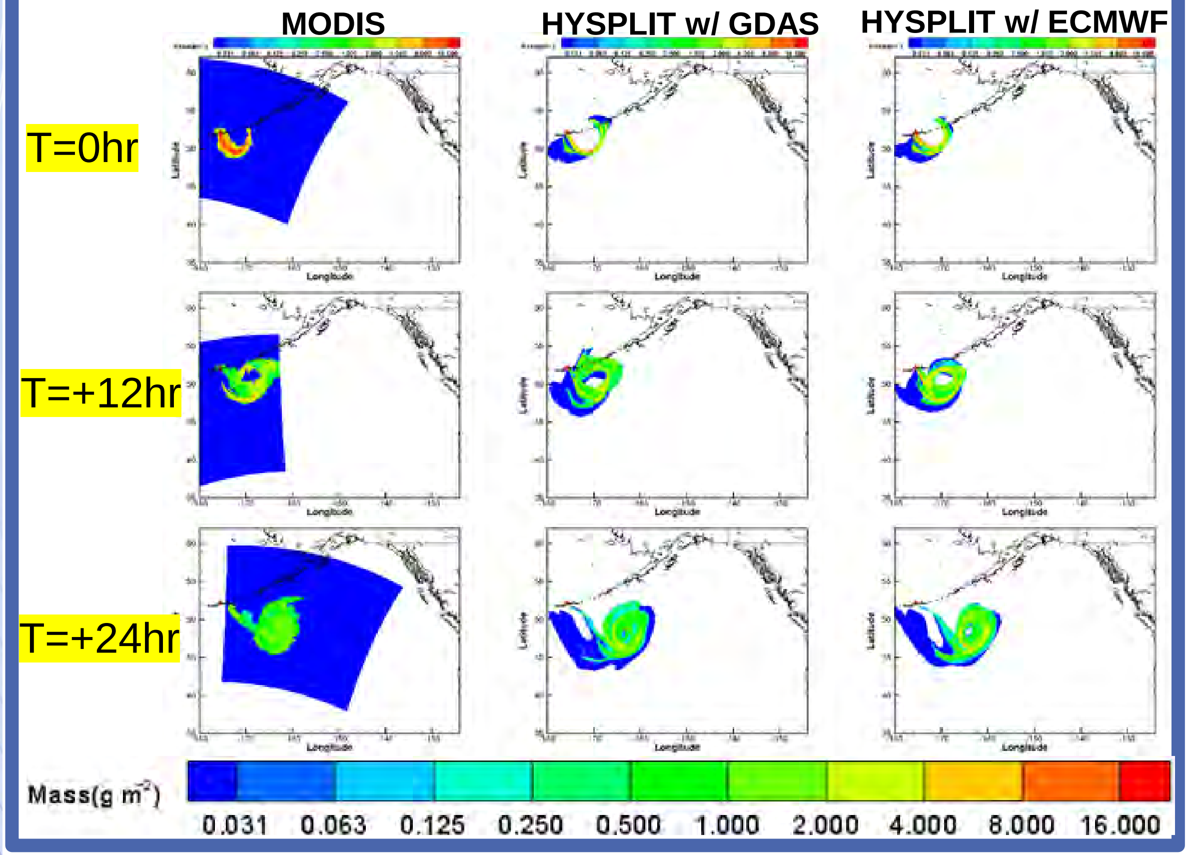

Unit emission simulation Bq/m$^3$
(HYSPLIT)



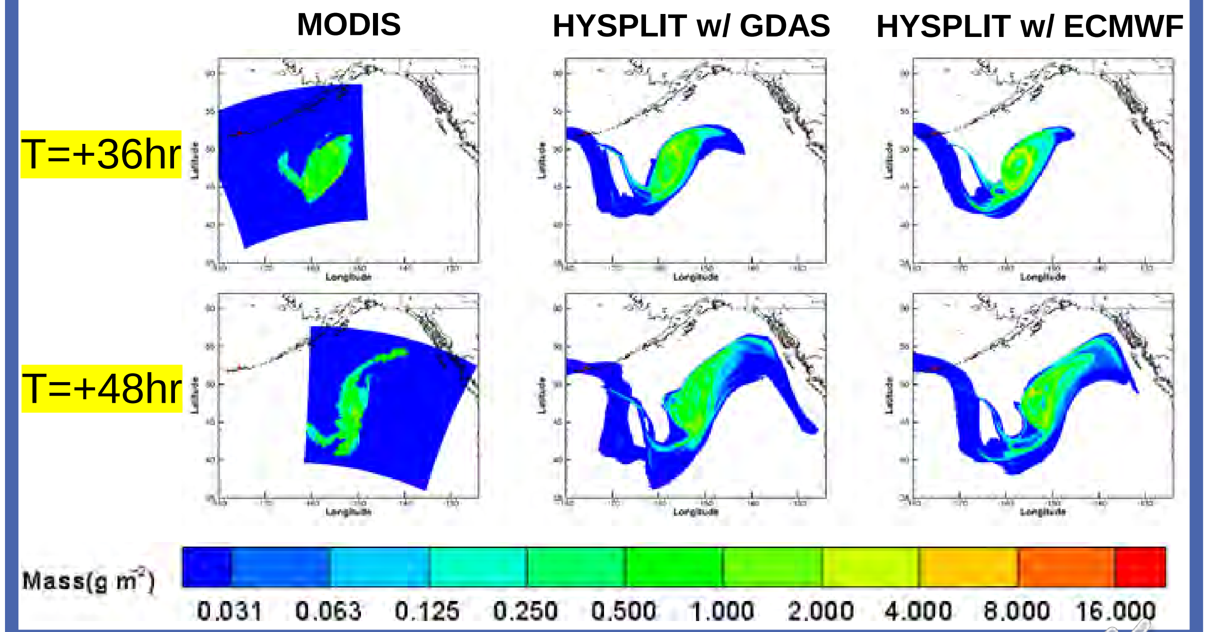

Estimated Cs-137 emissions Bq/h
(HEIMS)

# Volcanic ash application: Kasatochi eruption

Three sets of MODIS volcanic ash mass loading observations (~12 hours apart) are assimilated to generate ash emission estimates that have the best match between HYSPLIT simulations and MODIS observations.



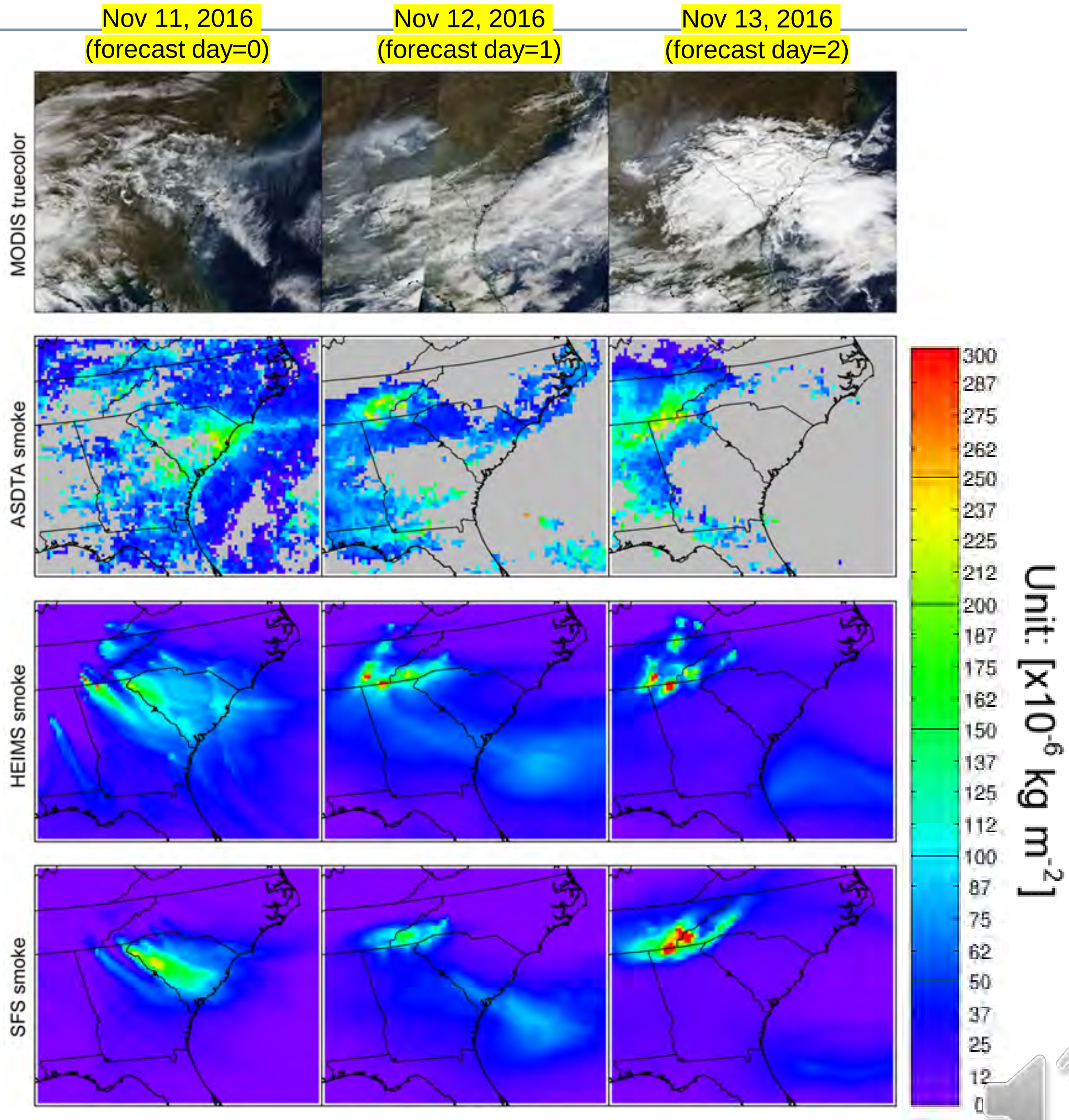

Hindcasts made with the estimated volcanic emissions that utilized MODIS observations at T=0, +12, and +24 hours.




Reference: Chai et al., 2017

# HYSPLIT-based Emission Inverse Modeling System for wildfires (HEIMS-fire)

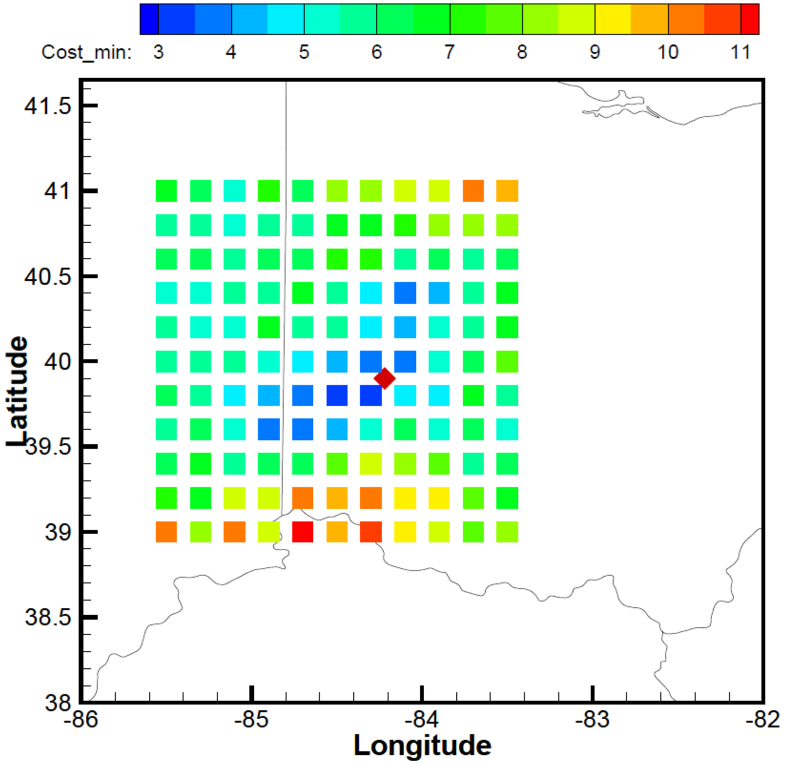
- Wildfire emission inversion system HEIMS-fire has been built based on the HYSPLIT model, a transfer coefficient matrix (TCM) and a cost function.
- High-temporal-resolution geostationary satellite smoke products are used in the inverse modeling.
- A case study for a large 2016 wildfire event in the Southeast U.S. using GOES data shows good performance, comparable to the current operational smoke forecasting system (SFS). Reference: Kim et al. (2020), *ACP* **20**: 10259
- Figure shows observed and forecasted smoke.
    - *Row 1:* true-color image from MODIS
    - *Row 2:* satellite-derived Automated Smoke Detection and Tracking Algorithm (ASDTA) smoke
    - *Row 3:* HEIMS smoke hindcast
    - *Row 4:* operational Smoke Forecast System (SFS)




Reference: Kim et al., 2020

# HYSPLIT inverse modeling study using CAPTEX data

Known emissions rates and emissions locations from the Cross Appalachian Tracer Experiment (CAPTEX) are used to test the HYSPLIT inversion system.




Minimum cost function of 121 potential source locations accurately shows location of tracer release (red diamond).

Table below shows for each CAPTEX release:

- Actual and estimated source location
- Δ = distance between actual and estimated source locations
- Actual release rate,
- $q_{min}$ = estimated release rate with unknown source location
- q' = estimated release rate with known source location
- $\epsilon_{q'}$ = uncertainty of estimated emissions rate

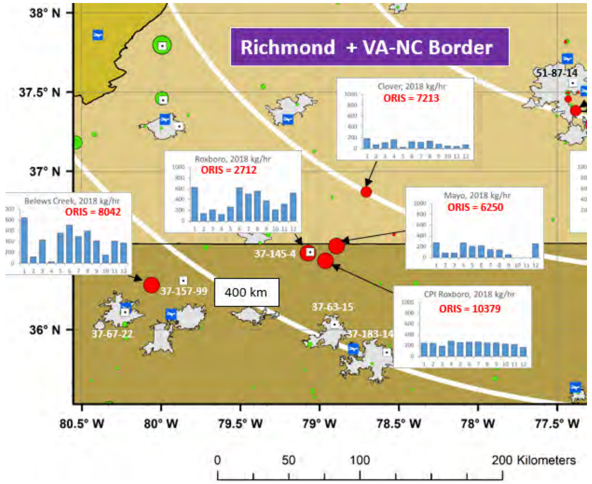
| | Source location (latitude, longitude) | | Δ(km) | Release rate (kg h$^{-1}$) | | | |
|---|---|---|---|---|---|---|---|
| No. | Actual | Estimated | | Actual | $q_{min}$ | $q'$ | $\epsilon_{q'}$ |
| 1 | 39.80°, −84.05° | 41.0°, −83.9° | 134.2 | 69.3 | 23.9 | 106.3 | 6.2 |
| 2 | 39.90°, −84.22° | 39.8°, −84.5° | 26.4 | 67.0 | 48.5 | 61.5 | 1.8 |
| 3 | 39.90°, −84.22° | 40.8°, −85.3° | 135.8 | 67.0 | 63.4 | 41.7 | 2.6 |
| 4 | 39.90°, −84.22° | 40.2°, −85.5° | 114.1 | 66.3 | 185.7 | 75.1 | 4.6 |
| 5 | 46.62°, −80.78° | 46.2°, −81.0° | 49.7 | 60.0 | 72.9 | 42.6 | 3.0 |
| 7 | 46.62°, −80.78° | 47.4°, −81.2° | 92.5 | 61.0 | 201.0 | 66.0 | 3.9 |

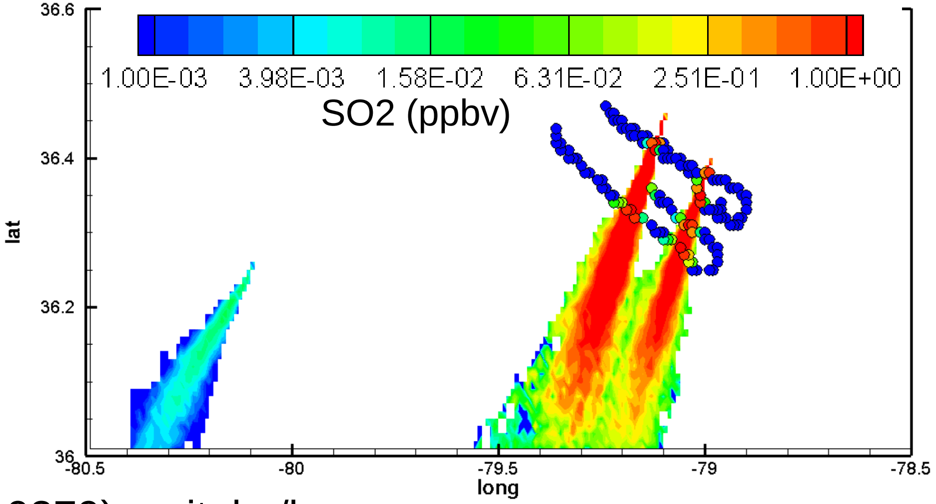
Reference: Chai et al., 2018

# HYSPLIT inverse estimated $SO_2$ emissions from power plants

Tracers of opportunity (known emissions from power plants with Continuous Emissions Monitoring systems) are used to test the HYSPLIT inversion system. Aircraft observations made downwind of power plants.


**Flight observations:**
Averaging: 1 minute
Altitude: 750-1250m;
Time: 19-21Z, 3/26/19



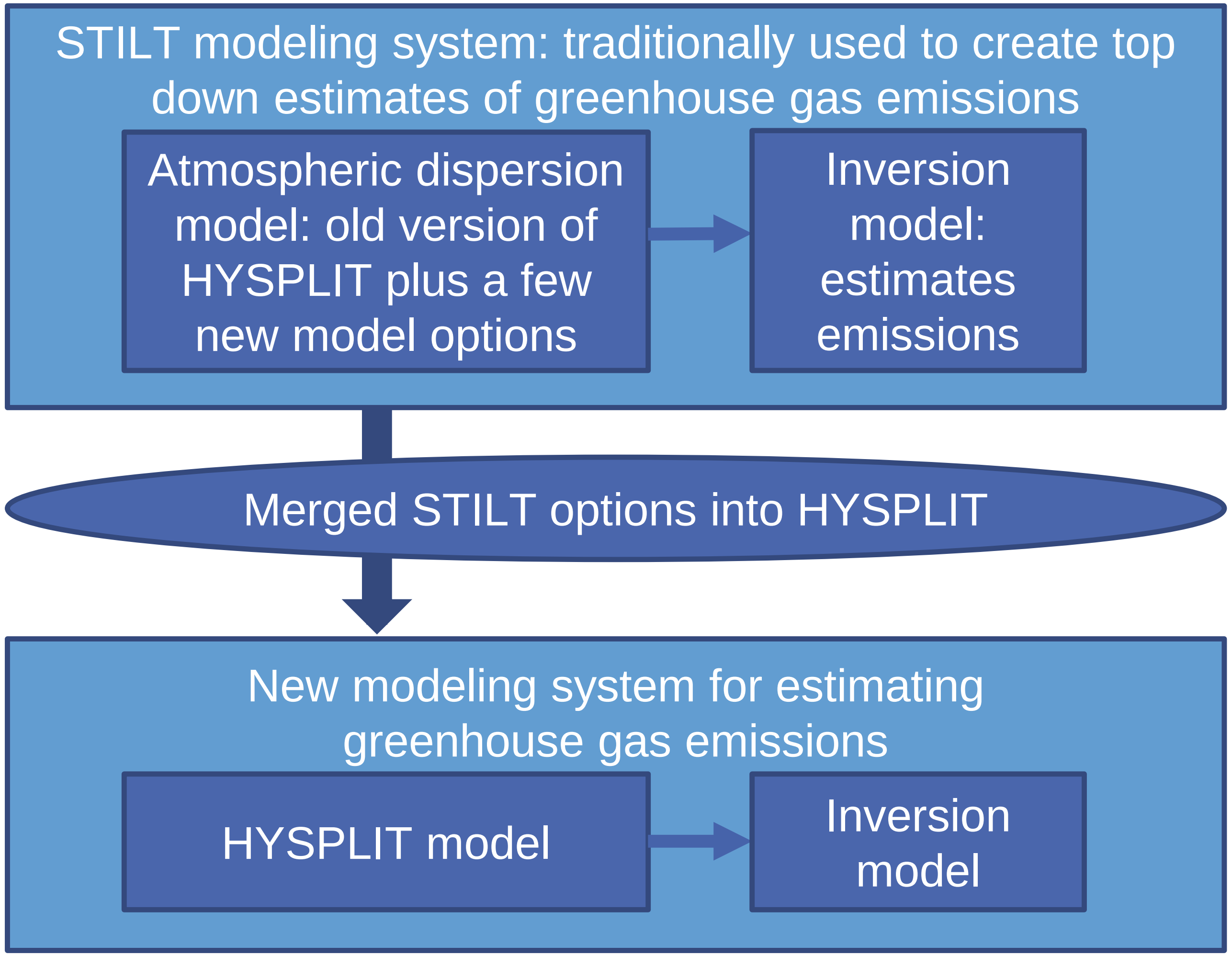

$SO_2$ Emission inversion results at Roxboro (#2712) and CPI Roxboro (#10379), unit: kg/hr

| #2712 | 15:00Z | 16:00Z | 17:00Z | 18:00Z | 19:00Z | 20:00Z | 21:00Z | Average |
|---|---|---|---|---|---|---|---|---|
| CEMs | **582** | **345** | **360** | **(509)** | **465** | **486** | **508** | **458** |
| Inverse | 292 | 363 | 0 | - | 867 | 237 | 0 | 293 |

| #10379 | 15:00Z | 16:00Z | 17:00Z | 18:00Z | 19:00Z | 20:00Z | 21:00Z | Average |
|---|---|---|---|---|---|---|---|---|
| CEMs | **281** | **300** | **279** | **(302)** | **316** | **295** | **293** | **294** |
| Inverse | 122 | 70 | 787 | - | 173 | 85 | 211 | 241 |

First guess: 1 Kg/hr , with uncertainty of 1E5 kg/hr (assuming CEMs unknown), Metric variable: Log(Mixing ratio)

# Expanding HYSPLIT capabilities for estimating greenhouse gas emissions




STILT options incorporated into HYSPLIT:

- Transport and dispersion module
- Vertical interpolation scheme
- Boundary layer turbulence parameterization
- Lagrangian timescale estimate
- Mixed-layer height estimation
- Two new convection schemes

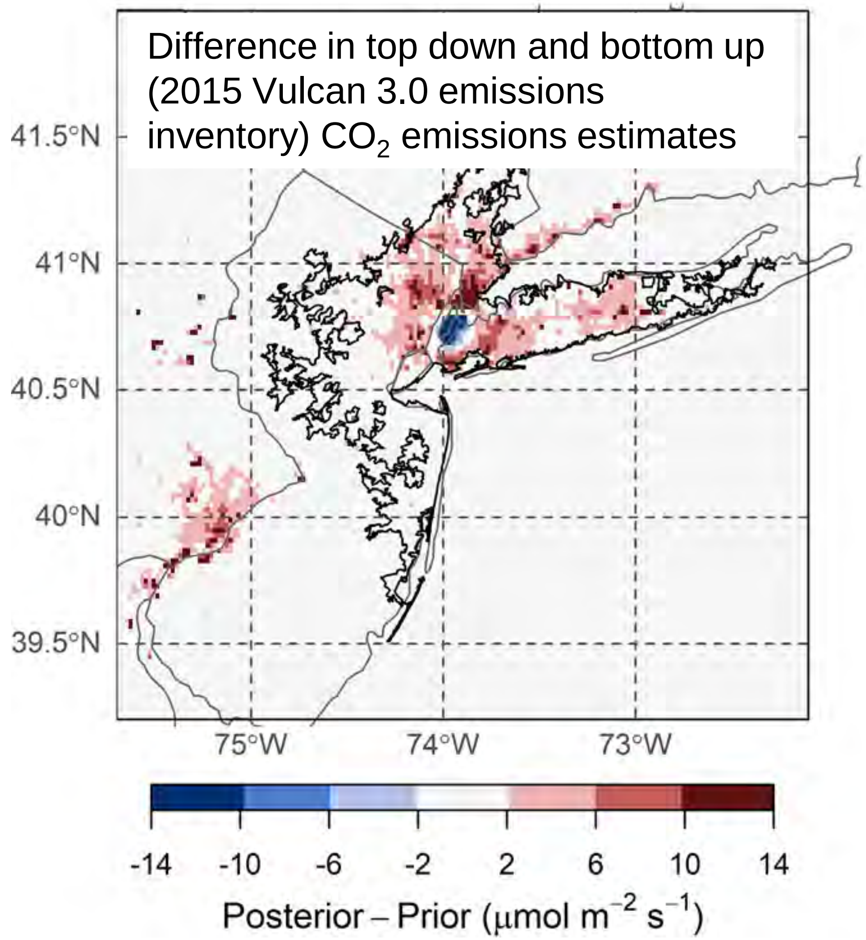
Benefits:

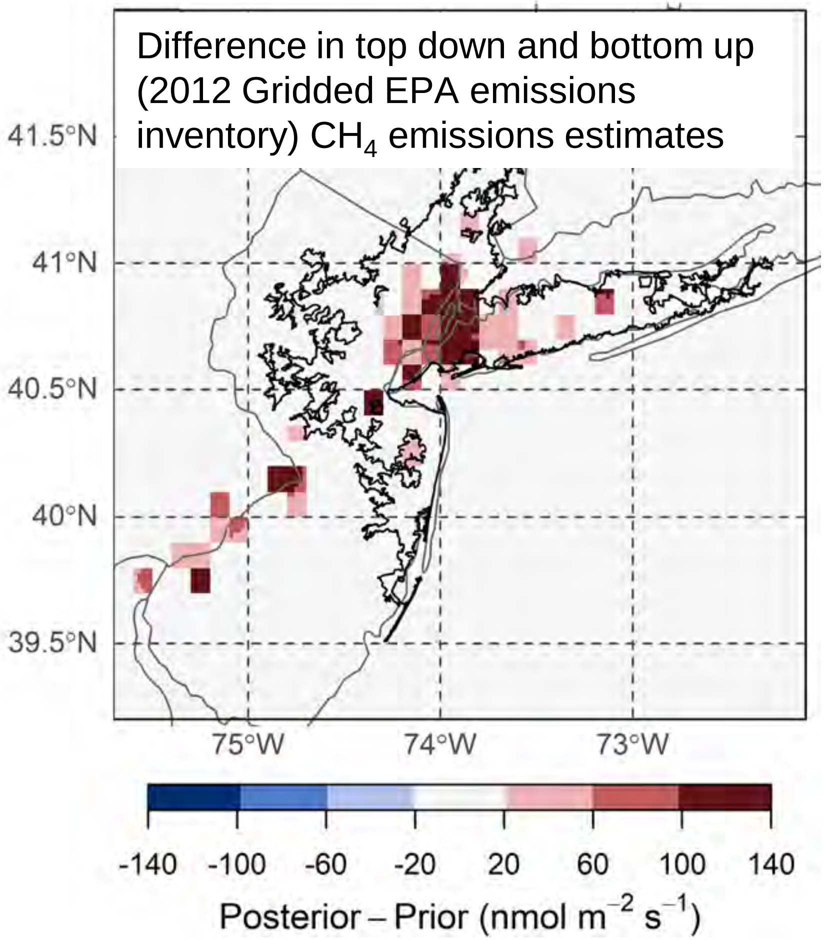
- Expands HYSPLIT options
- Ensures STILT routines are maintained and kept up to date

Reference: Loughner et al., 2021

# Example of new greenhouse gas inversion modeling system estimating $CO_2$ and $CH_4$ emissions in NYC

- Ensemble of backward HYSPLIT simulations with new STILT schemes performed along flight tracks of research flights during the non-growing seasons of 2018-2020 measuring $CO_2$ and $CH_4$ around New York City.
- HYSPLIT model results used within a Bayesian inverse modeling framework to estimate $CO_2$ and $CH_4$ emissions for the New York City metropolitan area.



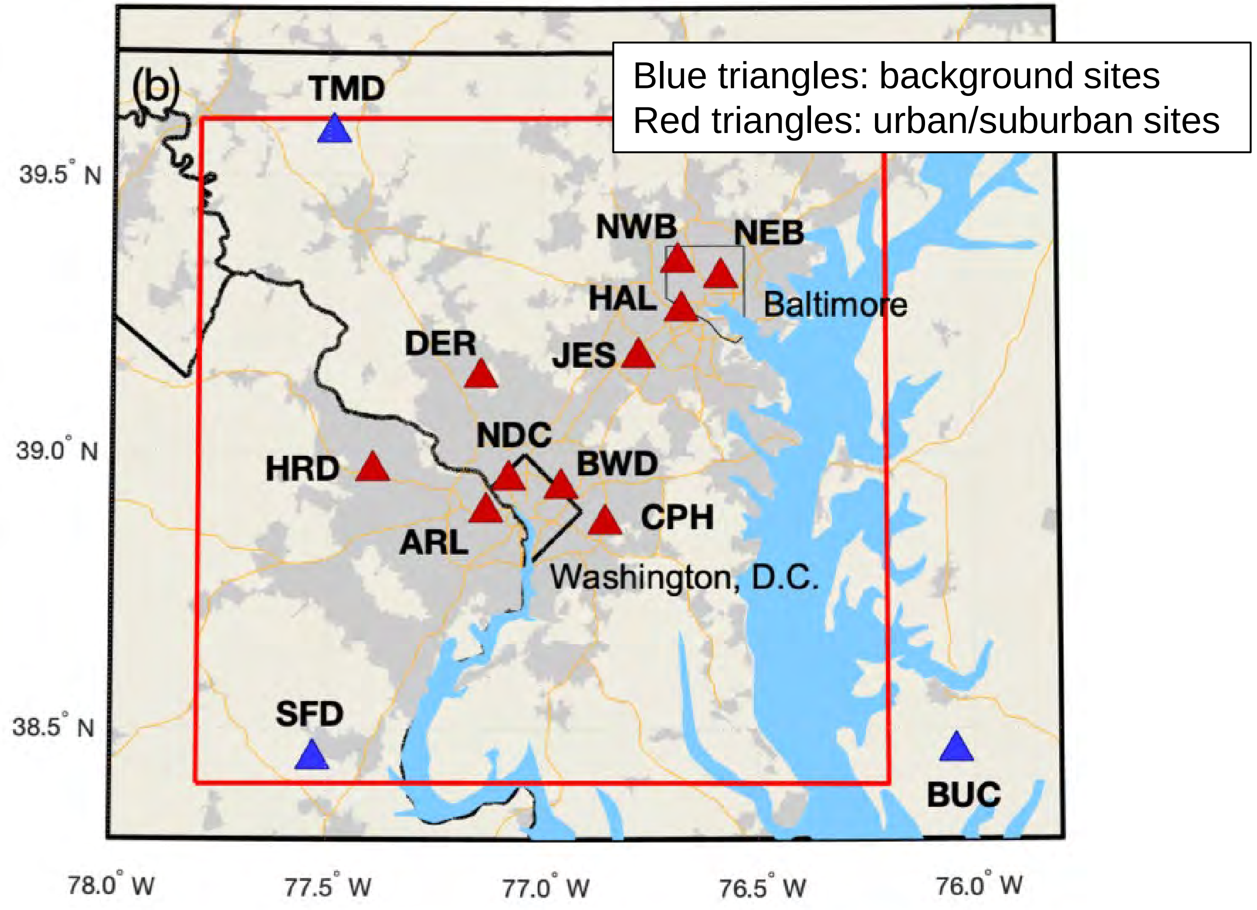

Reference: Pitt et al., 2022

# New greenhouse gas inversion modeling system being applied to for the Washington, DC – Baltimore, MD metropolitan area

- NIST tower-based greenhouse gas observation network in place throughout the Northeast Corridor with numerous sites in the Washington, DC – Baltimore, MD metropolitan area.

- Backward HYSPLIT simulations run from the measurement locations are being used within a Bayesian inversion framework to estimate $CO_2$ and $CH_4$ emissions.

NIST tower locations



# Publications


2017 Chai, T., A. Crawford, B. Stunder, M.J. Pavolonis, R. Draxler, and A. Stein. Improving volcanic ash predictions with the HYSPLIT dispersion model by assimilating MODIS satellite retrievals. *Atmos. Chem. Phys.*, 17, 2865-2879 (doi:10.5194/acp-17-2865-2017).

2018 Chai, T., A. Stein, and F. Ngan. Weak-constraint inverse modeling using HYSPLIT Lagrangian dispersion model and Cross Appalachian Tracer Experiment (CAPTEX) observations – Effect of including model uncertainties on source term estimation, *Geosci. Model Dev.*, 11, 5135-5148 (doi:10.5194/gmd-11-5135-2018).

2020 Angevine, W.M., J. Peischl, A. Crawford, C.P. Loughner, I.B. Pollack, and C.R. Thompson. Errors in top-down estimates of emissions using a known source. *Atmospheric Chemistry and Physics*, 20, 11,855-11,868 (doi:10.5194/acp-20-11855-2020).

2020 Kim, H.C., T. Chai, A. Stein, and S. Kondragunta. Inverse modeling of fire emissions constrained by smoke plume transport using HYSPLIT dispersion model and geostationary satellite observations. *Atmos. Chem. Phys.*, 20, 10259–10277 (doi:10.5194/acp-20-10259-2020).

2021 Loughner, C.P., Fasoli, B., A.F. Stein, and J.C. Lin. Incorporating features from the Stochastic Time-Inverted Lagrangian Transport (STILT) model into the Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model: a unified dispersion model for time-forward and time-reversed applications. *Journal of Applied Meteorology and Climatology*, 60, 799-910 (doi:10.1175/JAMC-D-20-0158.1).

2022 Pitt, J.R., I. Lopez-Cotez, K.D. Hajny, J. Tomlin, R. Kaeser, T. Jayathne, B.H. Stirm, C.R. Floerchinger, C.P. Loughner, C.K. Gately, L.R. Hutyra, K.R. Gurney, G.S. Roest, J. Liang, S. Gourdji, A. Karion, J.R. Whetstone, and P.B. Shepson. New York City greenhouse gas emissions estimated with inverse modelling of aircraft measurements, *Elementa Science of the Anthropocene*, 10(1), (doi:10.1525/elementa.2021.00082).

# Presentations

- Chai, T., M. Coheh, and F. Ngan (2021), Comparison of forward and backward source-receptor sensitivities for atmospheric inverse modeling using the HYSPLIT model with the Cross-Appalachian Tracer Experiment (CAPTEX) field experiment measurements, CTBT (Comprehensive Nuclear-Test-Ban Treaty) Science and Technology 2021 Conference, Vienna, Austria.
- Chai, T., H. Kim, A. Stein, D. Tong, Y. Li, and S. Kondragunta (2020), Estimating biomass burning emissions with HYSPLIT-based emission inverse modeling system and GOES Advanced Baseline Imager (ABI) observations, 2020 AGU Fall Meeting, online.
- Chai, T., H. Kim, A. Stein, D. Tong, Y. Li, and S. Kondragunta (2020), A case study of the 2018 Camp Fire event using HYSPLIT-based emission inverse modeling system with GOES Advanced Baseline Imager (ABI) observations and other measurements for wildfire smoke forecasts, EGU General Assembly 2020, online, EGU2020-12525, https://doi.org/10.5194/egusphere-egu2020-12525.
- Chai, T., H. Kim, A. Stein, and S. Kondragunta (2020), Wildfire smoke forecasts using HYSPLIT-based emission inverse modeling system and GOES observations, JPSS/GOES-R Proving Ground/Risk Reduction Summit, College Park, MD, USA.
- Chai, T., X. Ren, M. Cohen, A. M. Ring, A. Crawford, C. P. Loughner, A. F. Stein, F. Ngan, W. T. Luke, P. Kelly, P. Stratton, R. R. Dickerson, A. Karion, I. Lopez Coto, J. R. Whetstone (2020), HYSPLIT inverse modeling using flight observations to estimate SO2, CO2, and NOx point source emissions, 100th American Meteorological Society Annual Meeting, Boston, MA.
- Chai, T., H. Kim, A. Stein, and S. Kondragunta (2019), Smoke forecasts using HYSPLIT-based emission inverse modeling system and NOAA GOES smoke products, 2019 Joint Satellite Conference, Boston, MA.
- Chai, T., A. Stein, and F. Ngan (2018), Effect of including model uncertainties in HYSPLIT inverse modeling, 2018 AGU Fall Meeting, Washington, DC.

# Presentations (continued)

- Chai, T., H. Kim, A. Stein, and S. Kondragunta (2018), Estimating smoke emissions by assimilating satellite observations with HYSPLIT model", by, 9th International Workshop on Air Quality Forecasting Research (IWAQFR), Boulder, CO.
- Chai, T., H. Kim, and A. Stein (2018), Estimating smoke emission using GOES satellite observations and HYSPLIT model, 17th Annual CMAS Conference, Chapel Hill, NC.
- Chai, T, F. Ngan, and A. Stein (2017), Data assimilation and inverse modeling with HYSPLIT Lagrangian dispersion model, Seventh International WMO Symposium on Data assimilation, Florianópolis, Brazil.
- Chai, T., H. Kim, A. Stein, F. Ngan, A. Crawford, B. Stunder, and M.J. Pavolonis (2017), Data assimilation and inverse modeling with HYSPLIT Lagrangian dispersion model and satellite data – Applications to volcanic ash and wildfire smoke predictions, 2017 NOAA Satellite Conference, New York, NY.
- Chai, T., A. Stein, and F. Ngan (2017), HYSPLIT Inverse Modeling: Investigation Using Cross Appalachian Tracer Experiment (CAPTEX) Data and Ensemble Dispersion Simulations, CTBT: Science and Technology 2017 Conference (SnT2017), Vienna, Austria.
- Kim, H., T. Chai, A. Stein, and S. Kondragunta (2018), A HYSPLIT-based fire emission inverse modeling system for smoke forecast, 2018 AGU Fall Meeting, Washington DC.
- Kondragunta, S., T. Chai, H. Kim, and A. Stein (2019), Wildfire smoke forecasts using HYSPLIT-based emission inverse modeling system and satellite observations, 2019 AGU Fall Meeting, San Francisco, CA.
- Loughner, C.P., B. Fasoli, A. Stein, J. Lin (2021), Evaluation of STILT features within HYSPLIT for the CAPTEX and ANATEX tracer experiments, 24$^{th}$ Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA.

# Presentations (continued)

- Loughner, C.P., A. Stein, J. Lin (2020), STILT features incorporated into the HYSPLIT model, Meteorology for nuclear emergencies and nonproliferation (MET) exchange meeting, Livermore, CA.
- Loughner, C.P., A. Stein, J. Lin (2020), Evaluation of STILT features incorporated into HYSPLIT, AMS Annual Meeting, Boston, MA.
- Loughner, C.P., A. Stein, and J. Lin (2019), STILT features merged into HYSPLIT, $CO_2$-Urban Synthesis and Analysis (CO2-USA) Workshop, Boston, MA.
- Loughner, C.P., A. Stein, and J. Lin (2019), Evaluation of recently added STILT features into HYSPLIT, 23rd Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA.
- Loughner, C.P., A. Stein, and J. Lin (2018), Incorporation of STILT features into HYSPLIT, $CO_2$ Urban Synthesis and Analysis ("$CO_2$-USA") Workshop, Salt Lake City, UT.
- Loughner, C.P., A. Stein, and J. Lin (2017), $CO_2$-USA ARL modeling system updates, $CO_2$ Urban Synthesis and Analysis ("$CO_2$-USA") Workshop, Gaithersburg, MD.
- Pappin, A., others, and T. Chai (2018), Application of Different Concentration-Response Functions to Estimate the Societal Benefits of Reducing PM2. 5 and NOx Emissions, The ISES-ISEE 2018 Joint Annual Meeting, Ottawa, Canada.
- Stein, A., T. Chai, and F. Ngan (2018), Using Tracer Experiment Data to Test and Evaluate the HYSPLIT Lagrangian Model Inverse System, 98th American Meteorological Society Annual Meeting, Austin, TX.

# Future Plans

- Perform spatially and temporally resolved top-down estimates of greenhouse gas emissions in urban areas.
- Utilize tracers of opportunity to evaluate inversion schemes.
- Optimize Bayesian inversion modeling framework within HYSPLIT modeling system.
- Explore innovative modeling methods to reduce computational time and improve model results, such as incorporating Gaussian Mixture Model within inversion framework.
- Continue to enhance TCM inversion framework to improve nuclear, volcanic ash, and wildfire forecasts.

# Reconstructed Cs-137 concentrations (Bq/m3) using inversion-estimated emissions from Fukushima NPP