Model Evaluation and Improvement

***Presenter:* Fantine Ngan**

***Other Team Members:* Alice Crawford, Mark Cohen**

NOAA Air Resources Laboratory

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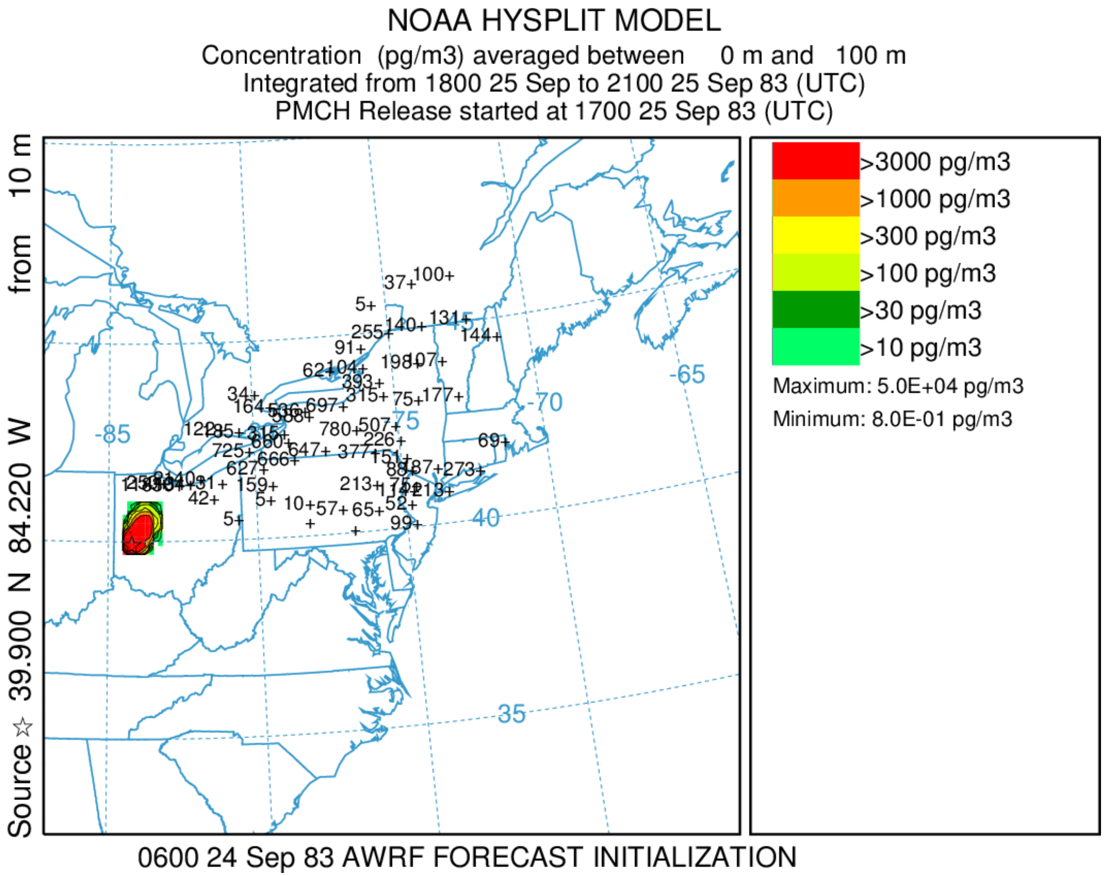
Model Evaluation and Improvement

- There are numerous sources of uncertainty in transport and dispersion modeling:
  - Emissions
  - Meteorology used to drive the HYSPLIT model
  - Model physics (e.g., horizontal and vertical mixing)
  - Model configuration (e.g., user-selected grid size)
- A fundamental part of our HYSPLIT model R&D involves comparison of simulation results with observations
- This allows us to assess how well the model is working and helps guide efforts to improve model performance
- We evaluate the HYSPLIT model using intentional tracer experiments, tracers of opportunity, and other observations
- We also evaluate the meteorological data used to drive the HYSPLIT model against observations, as this can be a significant source of uncertainty (e.g., wind speed and direction, stability, and mixing parameters)
- These model evaluation exercises help us to characterize, quantify and ultimately reduce uncertainties in HYSPLIT simulations



A HYSPLIT simulation of CAPTEX tracer experiment release #2 compared to tracer measurements

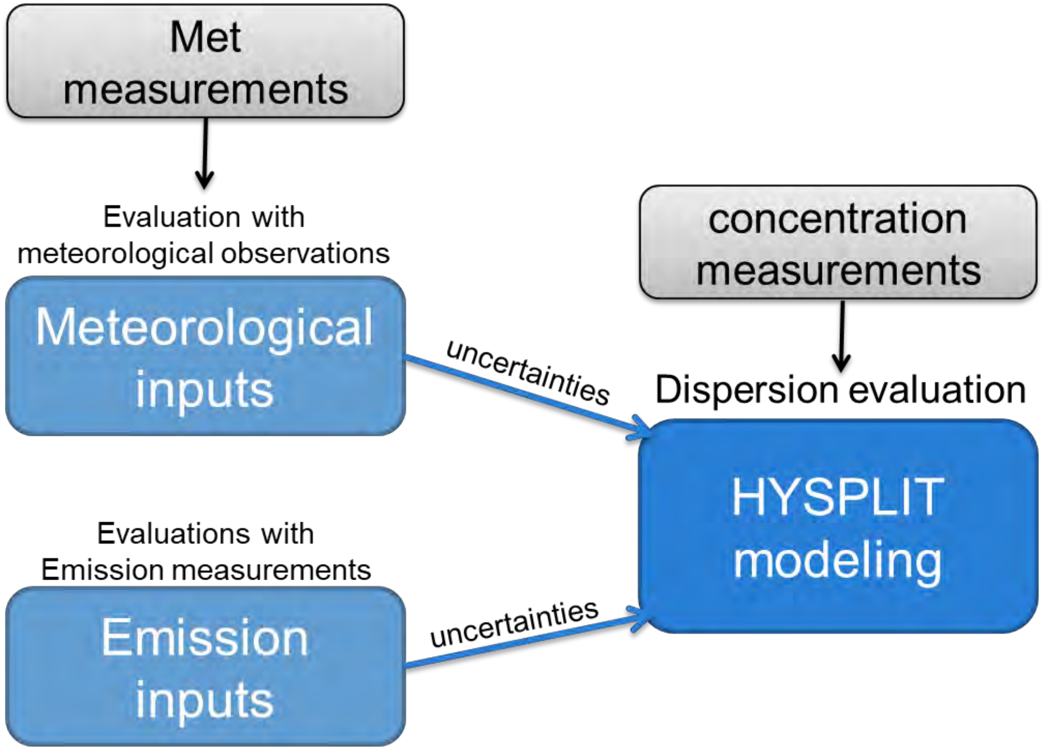
Relevance to OAR Strategic Goals

- *Design tools and processes to forecast high-impact weather, water, climate, ocean, and ecosystem events*

  -- OAR Strategy 2020-2026

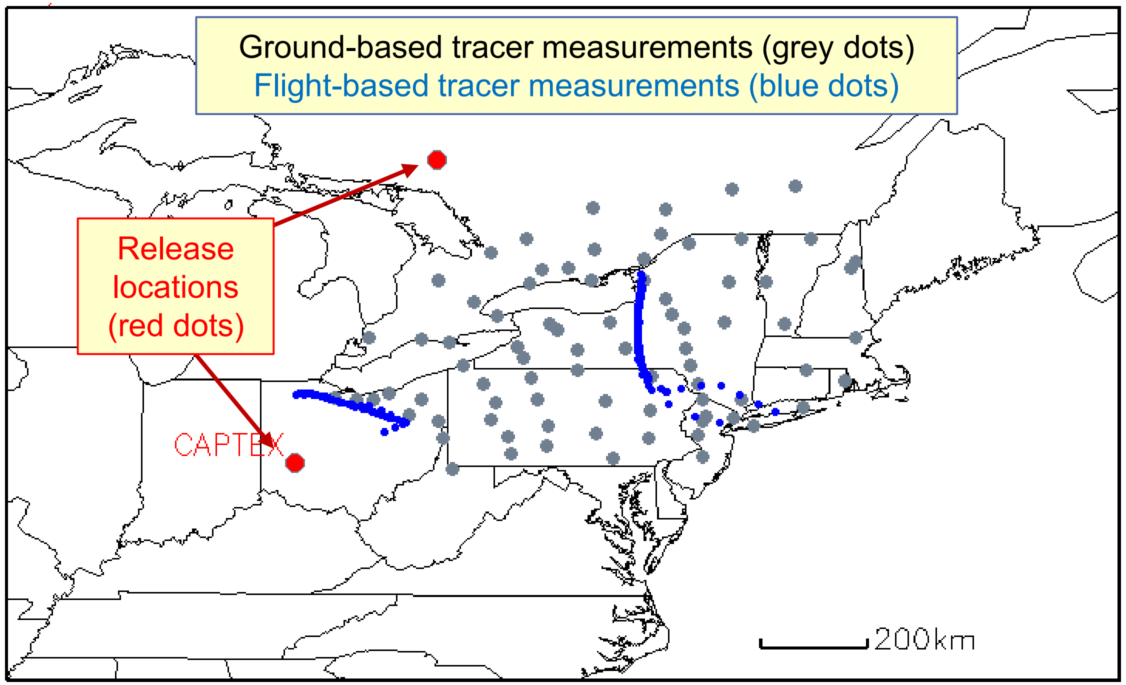
- *Improve weather & climate predictions by increasing our understanding of Planetary Boundary Layer (PBL) processes*

  -- OAR Implementation Plan 2021-2026

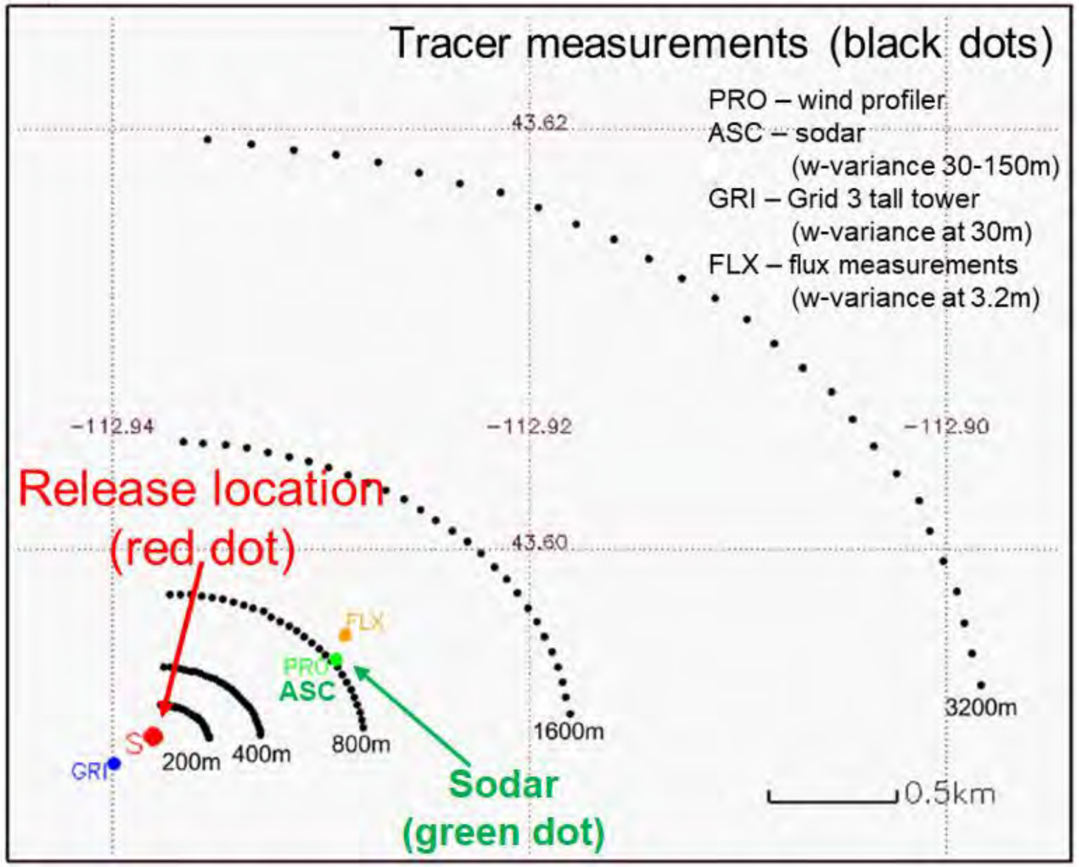


Tracer Experiments

Controlled tracer experiments use passive tracer releases (with known emission rate and location) and employ well-designed sampling networks for meteorological parameters and tracer concentration.



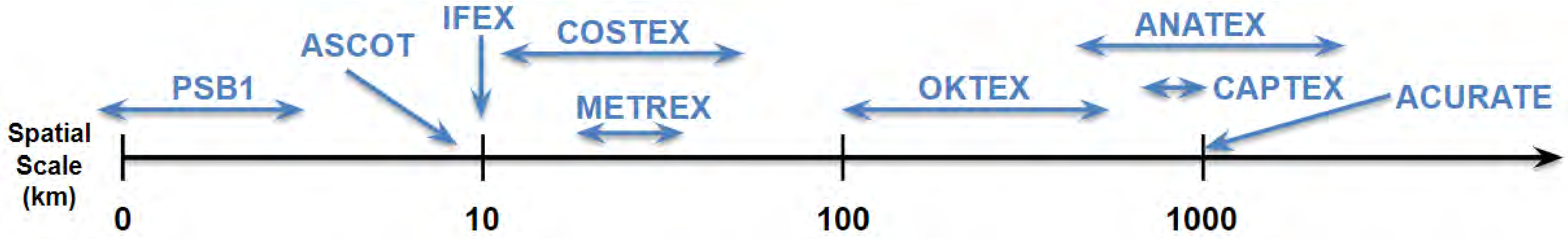
Tracer measurements (ground and flights) for CAPTEX 2 release.



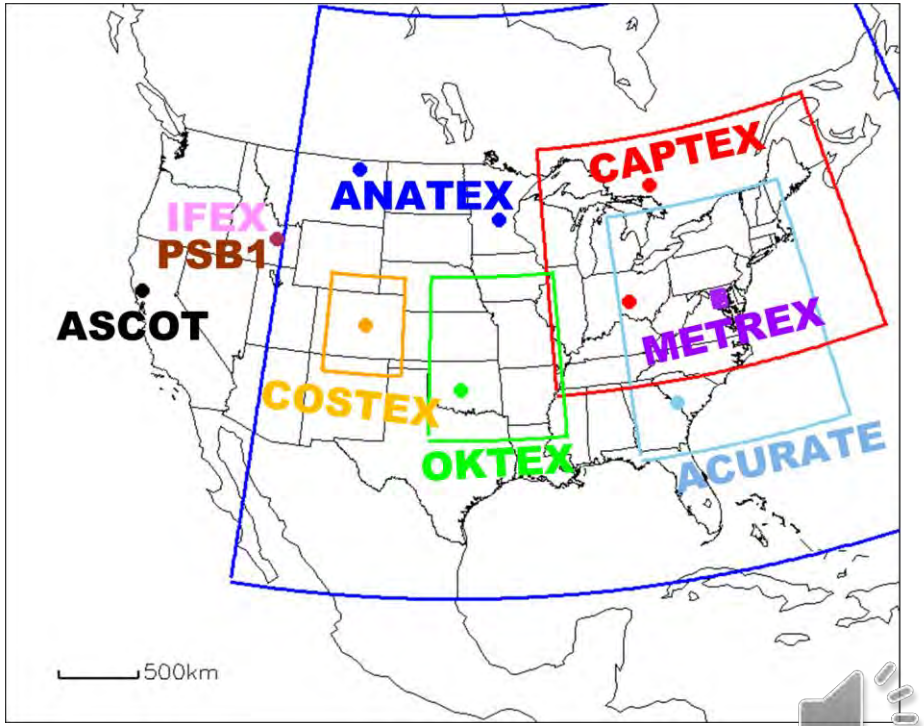
Sampling networks and meteorological measurements for Project Sagebrush Phase 1 (PSB1)

Tracer Experiments Conducted by ARL

Wide range of spatial scales in ARL tracer experiments, ranging from sub-kilometer to synoptic scale



- Atlantic Coast Unique Regional Atmospheric Tracer Experiment (**ACURATE**) – Savannah River Plant, SC, March 1982 through October 1983.
- Across North America Tracer EXperiment (**ANATEX**) – Glasgow, MT and St. Cloud, MN, January through March 1987
- Cross APpalachian Tracer EXperiment (**CAPTEX**) – Dayton, OH and Sudbury, ONT, September through October 1983
- OKlahoma Tracer EXperiment (**OKTEX**) – Oklahoma City, OK, July 1980
- MEtropolitan Tracer EXperiment (**METREX**) – Rockville, MD and Vernon, VA, January 1984 through January 1985
- Colorado Springs Tracer Experiment (**COSTEX**) – Colorado Springs, CO, October 2010
- Idaho Field Experiment (**IFEX**) – Idaho Fall, ID, July 1981
- Atmospheric Studies in Complex Terrain (**ASCOT**) – Anderson Creek Valley, CA, September 1980
- Project Sagebrush Phase 1 (**PSB1**) – Idaho Fall, ID, October 2013



Meteorological analysis datasets in HYSPLIT compatible format

<u>North American Regional Reanalysis (NARR)</u>

NCEP Eta Model product, converted to HYSPLIT format, 32-km, 3-hour and CONUS, 1979 – 2019

<u>Global Reanalysis (GBL)</u>

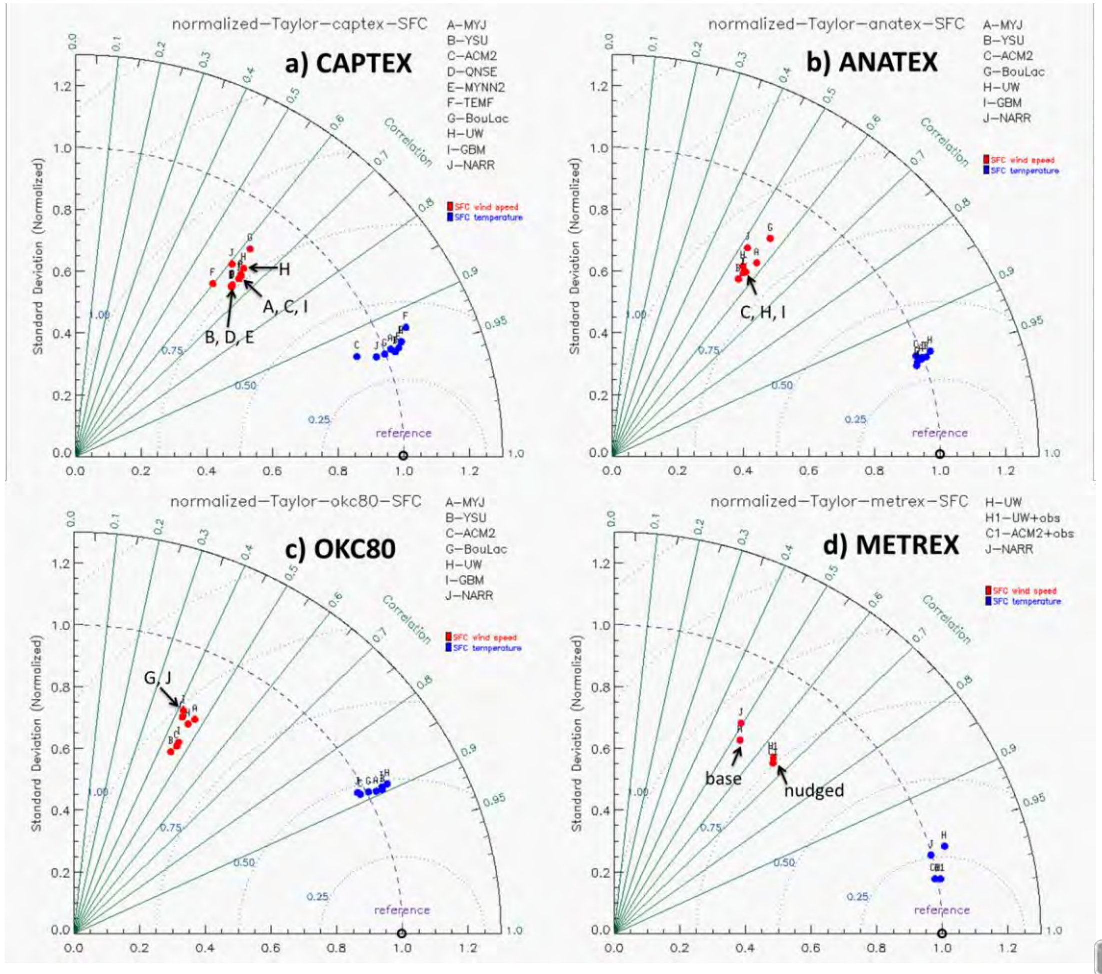
NCEP/NCAR Reanalysis Project, converted to HYSPLIT format, 2.5 deg, 6-hourly and global, 1948 – present year

The two analysis datasets above do not have momentum flux that HYSPLIT needs to diagnose some mixing parameters, so we have generated a new, long-term meteorological analysis dataset for research and development

<u>WRF analysis dataset</u>

- WRF-ARW model output converted to HYSPLIT format
- Tailored for dispersion applications based on statistical evaluation of tracer experiments (see figures at right)
- *27-km, Hourly, CONUS, 1980 – present*
- *Available fields include: friction velocity, TKE, time-averaged wind fields, turbulent exchange coefficient*

Normalized Taylor diagrams of surface wind speed and temperature. (Ngan and Stein, 2017) Different WRF configurations were examined to see which provided the best data for dispersion modeling during various tracer experiments.



Data Archive of Tracer Experiments and Meteorology (DATEM)

- DATEM is an essential tool for HYSPLIT evaluation and development.
- Available to the public since the early 2000s.
- Available data include emissions, tracer measurements, and meteorological data (WRF recently added) for each tracer experiment.
- Evaluation tools allows users to assess HYSPLIT's performance themselves.
- DATEM benefits the dispersion modeling community, allowing sensitivity studies and model intercomparison studies to be carried out.

Examples of DATEM format and analytical results, for the CAPTEX tracer experiment

Tracer releases

\datem\exp_data\captex\emit-t1.txt

year	mn	dy	shr	dur	lat	lon	pmch
1983	09	18	1700	0300	39.80	-84.05	208000
1983	09	25	1700	0300	39.90	-84.22	201000
1983	10	02	1900	0300	39.90	-84.22	201000
1983	10	14	1600	0300	39.90	-84.22	199000
1983	10	26	0400	0300	46.62	-80.78	180000
1983	10	28	1530	0030	39.90	-84.22	32000
1983	10	29	0600	0300	46.62	-80.78	183000

Tracer concentrations

\datem\exp_data\captex\meas-t1.txt

year	mn	dy	shr	dur	lat	lon	pmch	stn
1983	09	18	1800	0300	39.65	-80.42	.0	302
1983	09	18	1800	0300	40.38	-80.63	.0	306
1983	09	18	1800	0300	40.77	-80.75	.0	308
1983	09	18	1800	0600	40.92	-81.43	.0	310
1983	09	18	1800	0300	41.30	-81.15	.0	312
1983	09	18	1800	0300	41.42	-81.87	.0	314
1983	09	18	1800	0300	41.30	-82.22	343.2	316
1983	09	18	1800	0300	41.27	-82.62	.0	318
1983	09	18	1800	0300	41.33	-83.12	.0	320
1983	09	18	1800	0600	40.00	-79.08	.0	402
1983	09	18	1800	0600	40.43	-79.15	.0	404
1983	09	18	1800	0600	41.63	-79.70	.0	410
1983	09	18	1800	0600	42.08	-80.18	.0	412
1983	09	18	1800	0600	42.60	-80.50	15.6	452
1983	09	18	1800	0600	42.67	-81.15	.0	454

Statistics summary

```
        captex_meas.txt     results file: statA.txt
Model variation:    Tracer number: 0   Station select: All
        ---------------------------------

   2280 Unaveraged data points for processing
   0.00 Percentile input for zero measured
   0.00 Zero measured concentration value

   0.38 Correlation coefficient (P=99%)
   0.28 Regression Slope
  19.46 T-value (|Slope|/Standard Error)
 213.14 Average measured concentration
 157.92 Average calculated concentration
   0.74 Ratio of calculated/measured
  51.67 Normalized mean square error
1318.81 Root mean square error
   2210 Number of pairs analyzed

 -55.23 Average bias [(C-M)/N]
-127.56 Lo 99 % confidence interval
  17.11 Hi 99 % confidence interval
  -0.30 Fractional bias [2B/(C+M)]

  28.15 False Alarm Rate [fa/(fa+hit)]
  54.46 Probability of Detection [hit/(hit+miss)]
  44.88 Threat Score [hit/(fa+hit+miss)]

  45.18 Fig of merit in space (%)

 -36.47 Factor exceeding [N(C>M)/N-0.5]
   4.80 Percent C/M ± 2
   9.41 Percent C/M ± 5
  11.72 Percent C/M ±10
  15.48 Percent M>0 and C>0
  12.71 Percent M>0 and C=0
  71.81 Percent M=0 and C>0

 686.40 Measured   95-th percentile
 218.40 Measured   90-th percentile
  15.60 Measured   75-th percentile
   0.00 Measured   50-th percentile

 666.06 Calculated 95-th percentile
 238.22 Calculated 90-th percentile
   0.00 Calculated 75-th percentile
   0.00 Calculated 50-th percentile

  11.00 Kolmogorov-Smirnov Parameter

   2.34 Final rank (C,FB,FMS,KSP)
```

Statistical Analysis

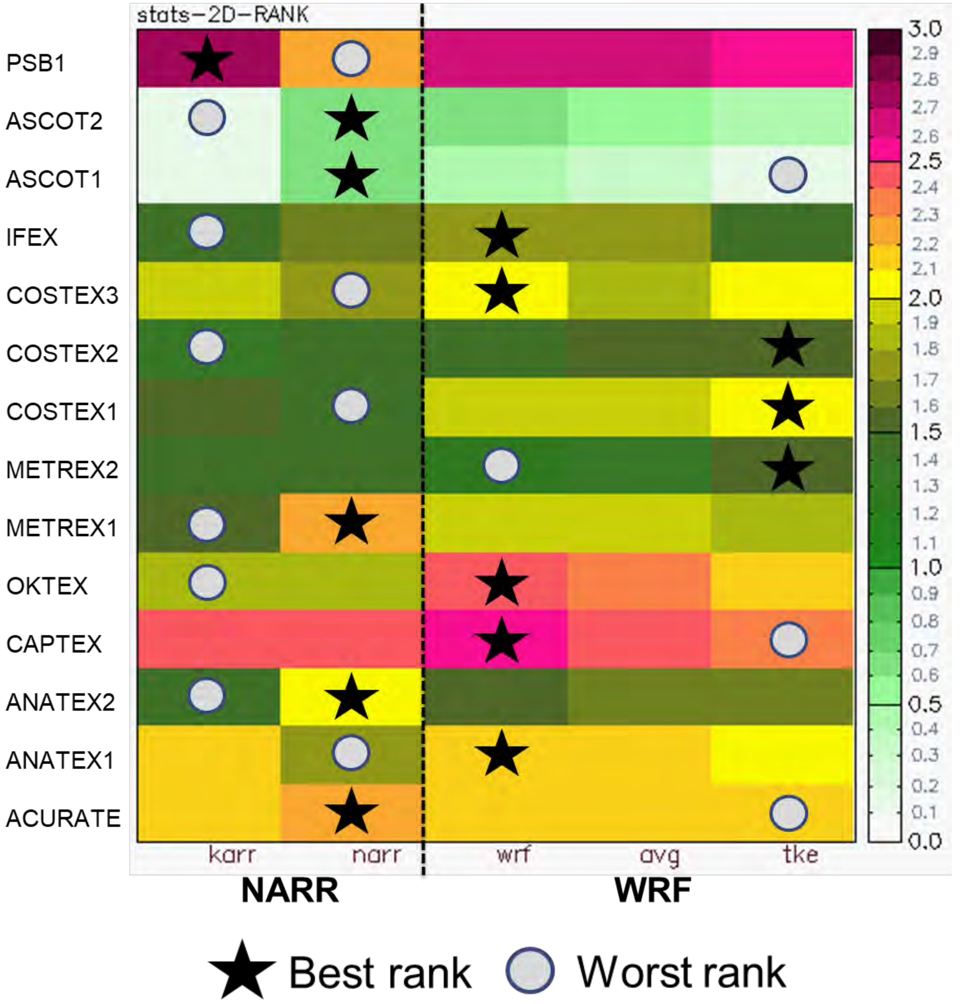
Statistical rank

Rank, a cumulative statistical score (range between 0-4)

$$rank = R^2 + 1 - \left|\frac{FB}{2}\right| + \frac{FMS}{100} + \left(1 - \frac{KSP}{100}\right)$$

R – Correlation coefficient
FB – Fractional bias
FMS – Figure of merit in space
KSP – Kolmogorov-Smirnov parameter

name	Met data	Model wind	HYSPLIT PBL stability	HYSPLIT mixing
karr	NARR	Instantaneous wind	Wind/Temp profiles	Kantha-Clayson
narr	NARR	Instantaneous wind	Wind/Temp profiles	TKE
wrf-kc	WRF	Instantaneous wind	Heat/momentum flux	Kantha-Clayson
wrf-avg	WRF	Time-averaged wind	Heat/momentum flux	Kantha-Clayson
wrf-tke	WRF	Time-averaged wind	Heat/momentum flux	TKE

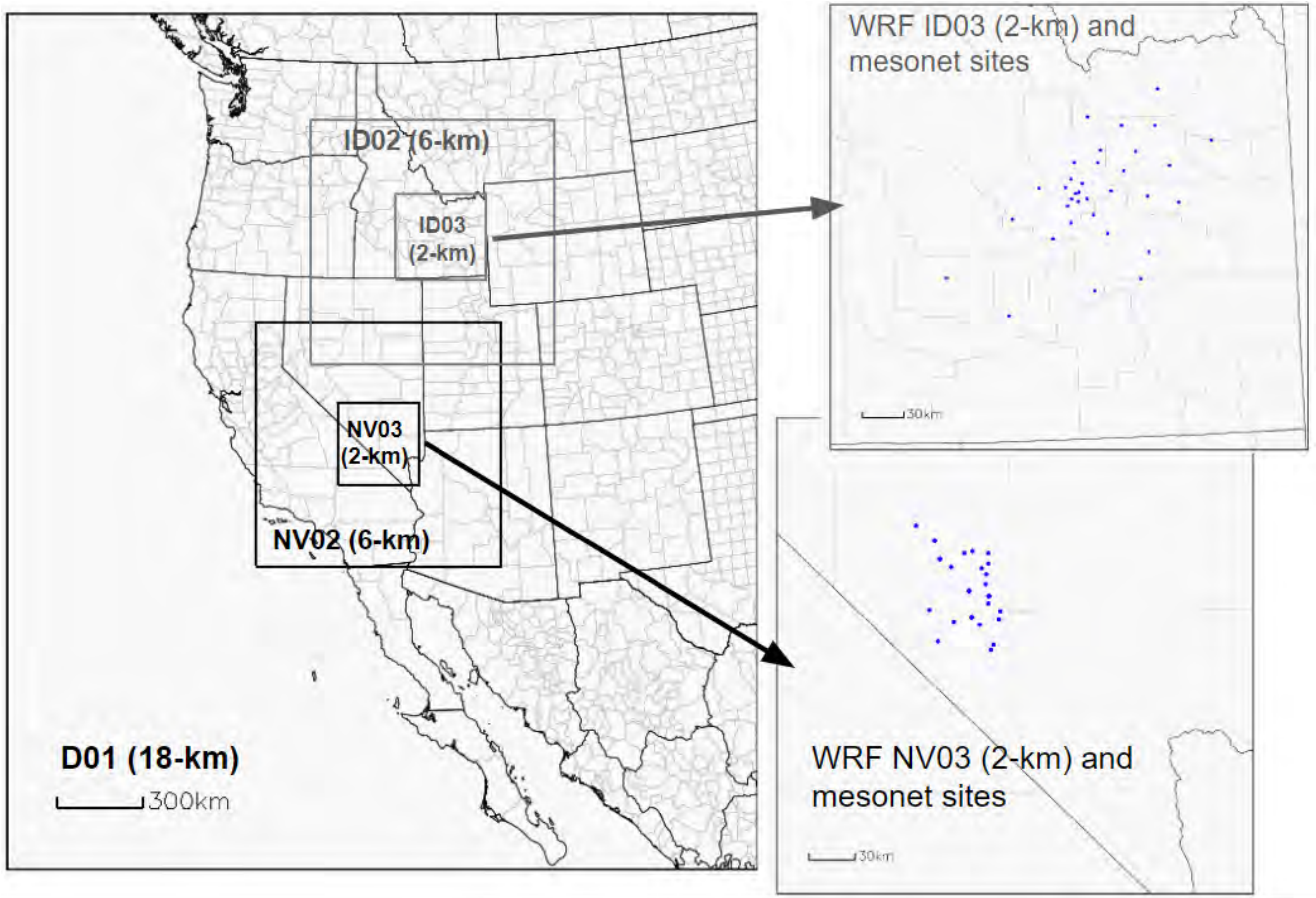


WRF Modeling Project for SORD and FRD

- An operational WRF modeling system to provide forecasts for daily operations, special experimental support, and emergency response components of the ARL Western Division missions (SORD and FRD).
- A coupling of modeling and measurements provides a platform to increase understanding of PBL dynamics, with attention to phenomena that impact the transport and dispersion of pollutants.
- The system will be a testbed for ARL research projects such as general PBL parameterizations, direct mesonet data inclusion, and the study of desert climate.
- The system has been operating since May 2021 to produce a 4-day forecast, every six hours.
- A web app was implemented to display the graphics for the daily use of the Western Divisions.

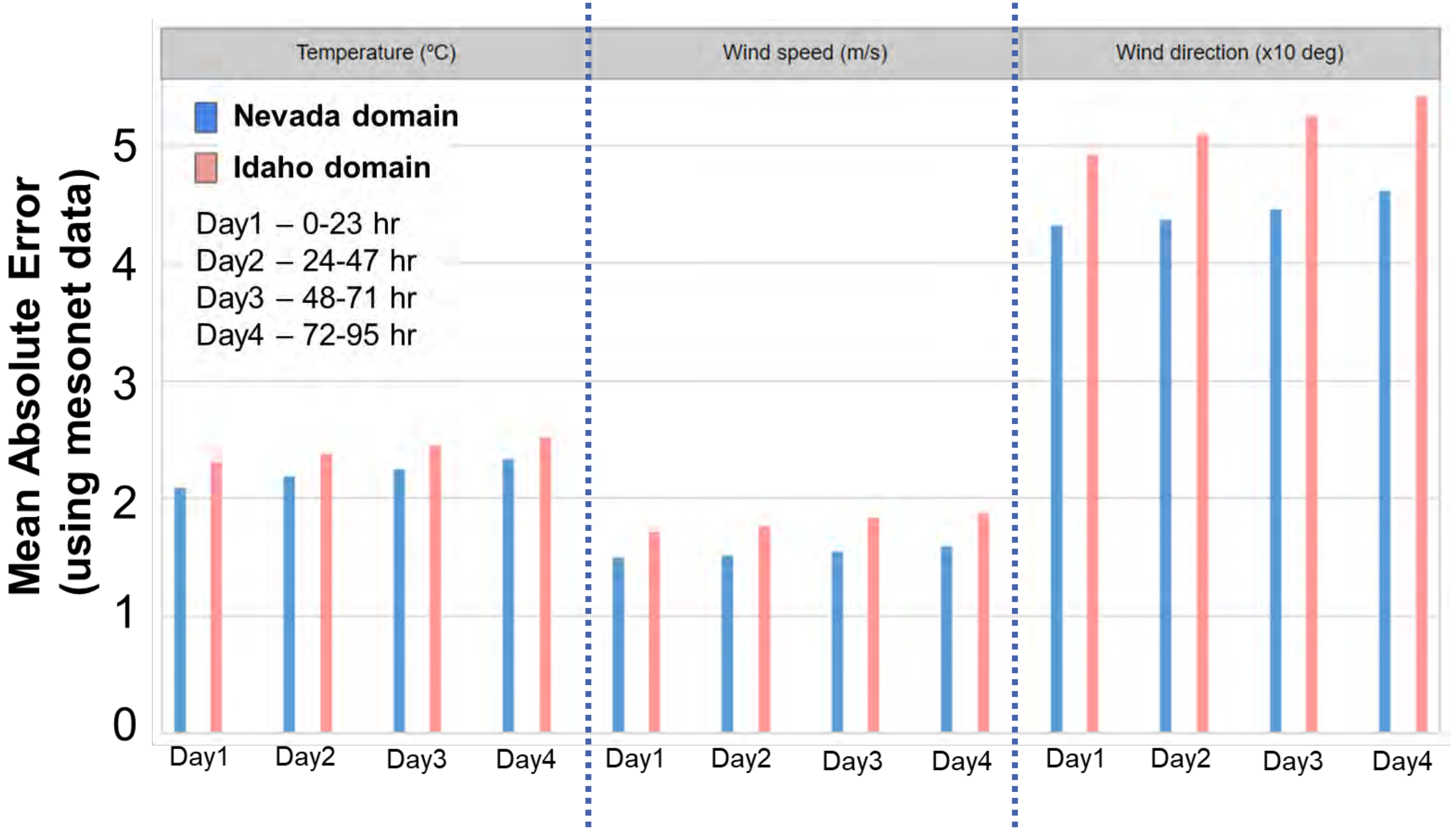
  https://apps.arl.noaa.gov/wrff/

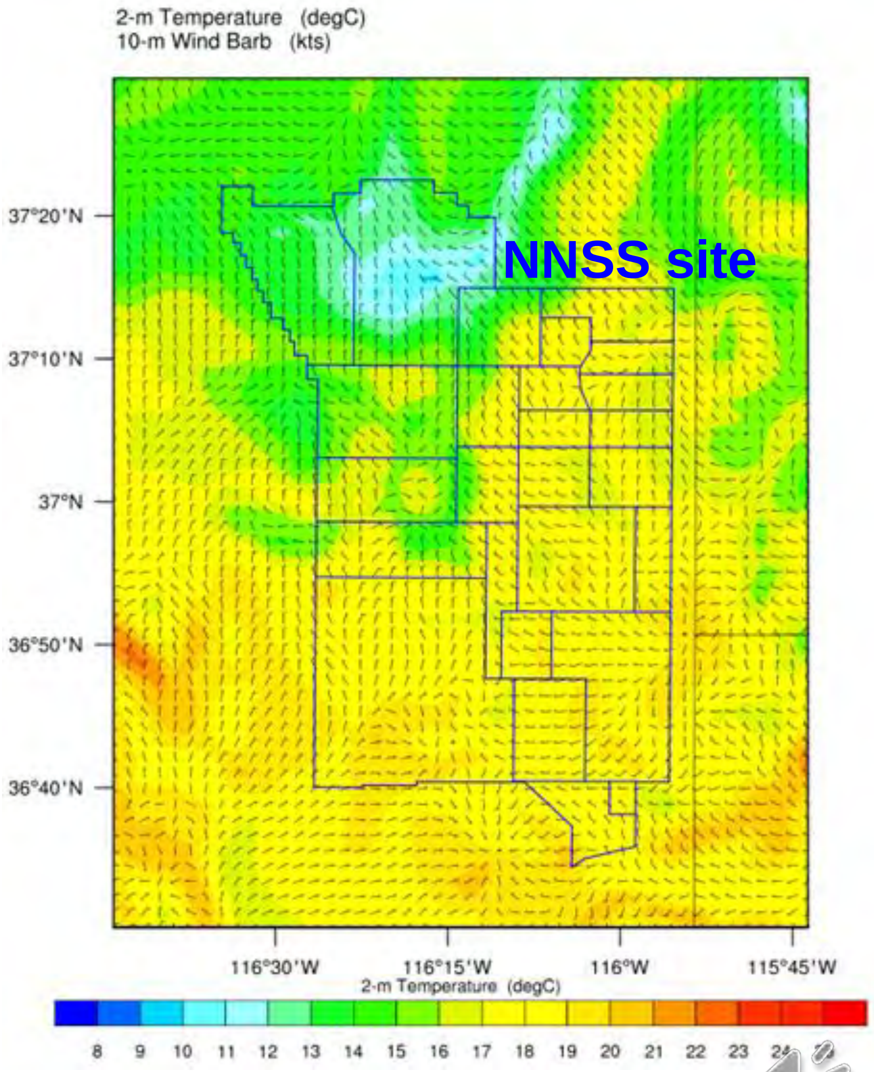
- Individual domains for Nevada area and Idaho regions, sharing the same 18-km outer domain.



Evaluation of the WRF Modeling Project

Six months of forecasting results were evaluated by comparison against the mesonet data collected by the ARL Western Divisions.

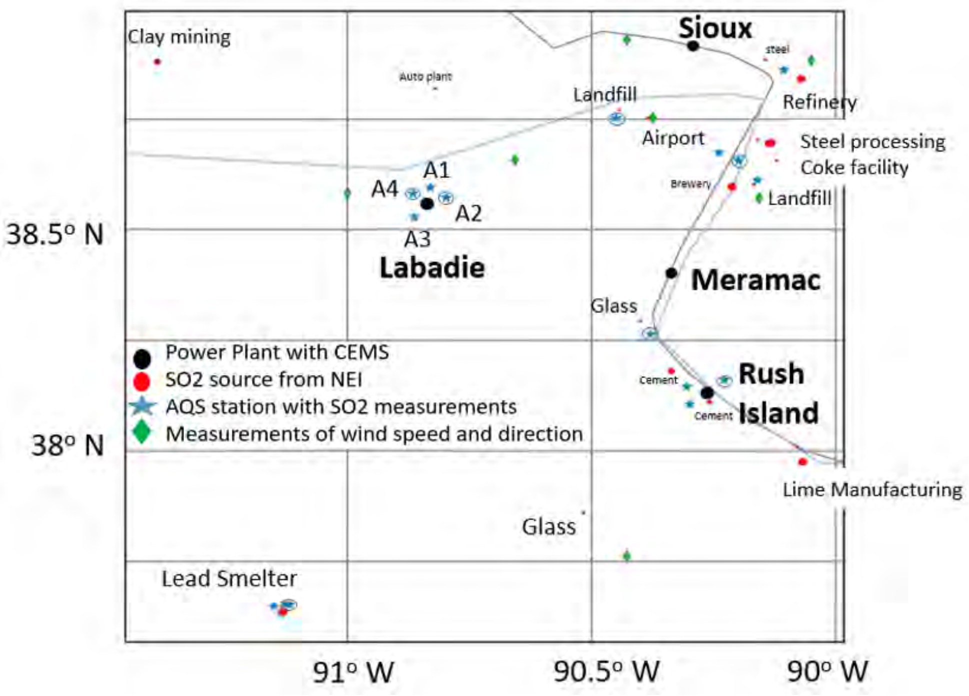




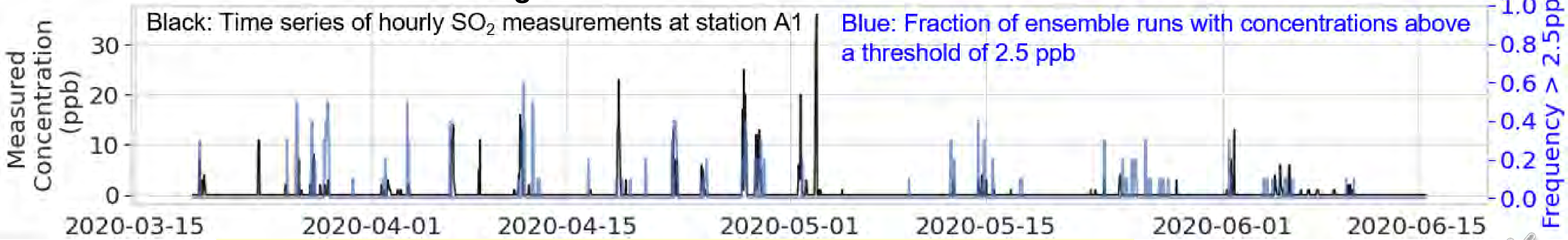
Tracers of Opportunity

- A *tracer of opportunity* can be any atmospheric release of a substance where the emissions rate has been measured or can be independently estimated, and for which downwind concentration measurements exist and/or which can be made.
    - industrial accidents (e.g., Fukushima nuclear accident)
    - natural processes (e.g., volcanic eruptions)
    - byproduct of industrial facilities (e.g., emissions from power plants)
- Example: SO_2 and CO_2 emissions from power plants -- emissions and downwind concentrations are measured; extended met measurements are also sometimes available (mesonets; Doppler Lidar, etc).
- Chemical transformations can be modeled or are relatively unimportant at time scales of less than a day (close to the source).

A study for the area around St. Louis, MO



An ensemble of 5 model runs using different met datasets

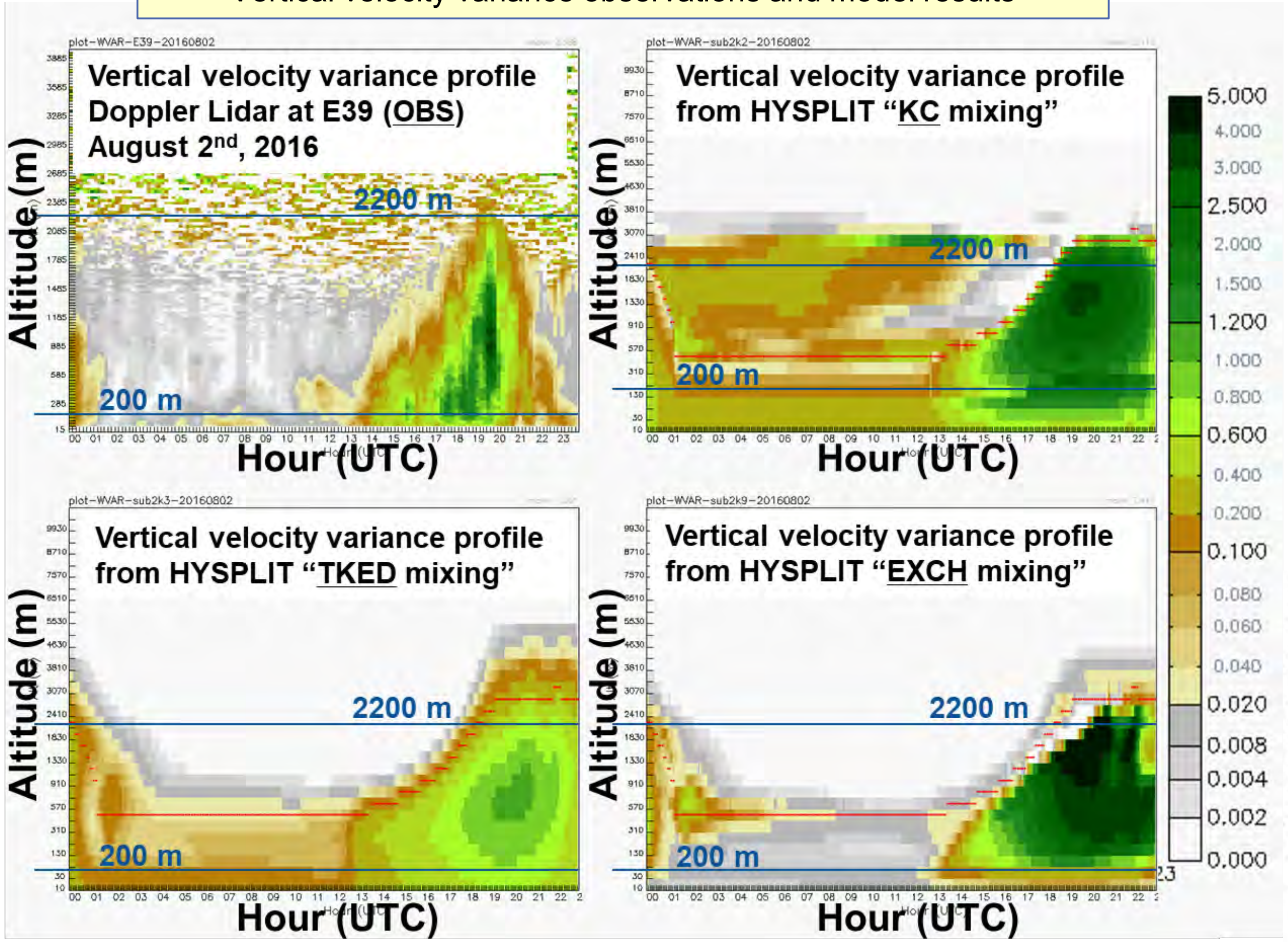


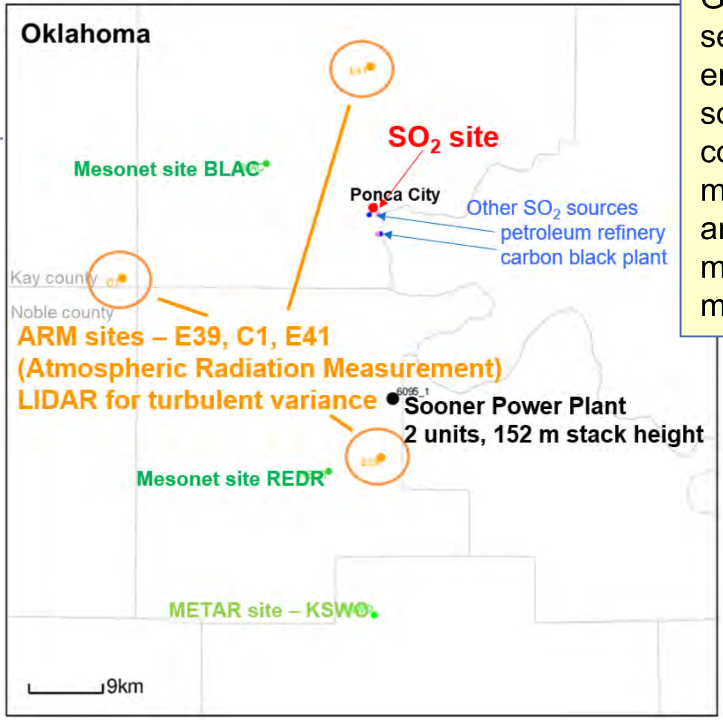
Peak modeled concentrations (not shown in this figure) were underpredicted, but the use of an using ensemble can improve the detection of peaks – for most of the observed peaks, at least one model-ensemble member showed a peak at or above 2.5 ppb.

Tracers of Opportunity

A study for the area around Ponca City, OK

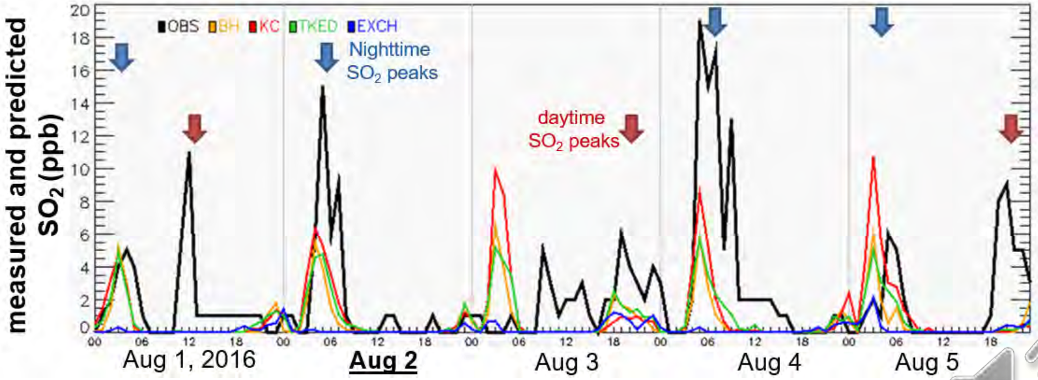
Vertical velocity variance observations and model results





Geographical setting of emissions sources, concentration measurements, and meteorological measurements

Modeled SO_2 concentrations (4 different mixing methods) and measurements



Quality and Performance: *Publications*

Pendergrass, W. R., F. Ngan, B. B. Hicks, R. P. Hosker, C. A. Mazzola, and D. A. Bruggeman, 2020: Demonstrating the Feasibility of Using the 1996 MVP Tracer Study for Transport and Diffusion Model Validation. NOAA Tech Memo OAR ARL-281. 50 pp.

Ngan, F., C. P. Loughner, and A. Stein, 2019: The evaluation of mixing methods in HYSPLIT using measurements from controlled tracer experiments. Atmos. Environ., 219, 117043.

Ngan, F., A. Stein, D. Finn, and R. Eckman, 2018: Dispersion simulations using HYSPLIT for the Sagebrush Tracer Experiment. Atmos. Environ., 186, 18-31.

Ngan, F., Stein, A., 2017. A long-term WRF meteorological archive for dispersion simulations: application to controlled tracer experiments. J. Appl. Meteor. Climatol. 56, 2203–2220. https://doi.org/10.1175/JAMC-D-16-0345.1.

Rolph, G., A. Stein, and B. Stunder, 2017: Real-Time Environmental Applications and Display System: READY. Environ. Modell. Software, 95, 210–228, doi:10.1016/j.envsoft.2017.06.025.

Quality and Performance: *Presentations*

- Ngan, F., A. Crawford, M. Cohen, C. Loughner, and A. Stein, 2020: Evaluation of turbulent mixing in HYSPLIT using a tracer of opportunity dataset. 100th AMS Annual Meeting, Boston, MA, AMS.
- Crawford, A. M. Cohen, F. Ngan, J. Heffter, B. Baker, W. T. Luke, and A. F. Stein, 2020: A Tracer of Opportunity Dataset for Atmospheric Transport and Dispersion Model Evaluation. 100th AMS Annual Meeting, Boston, MA, AMS.
- Cohen, M., A. Crawford, C. Loughner, W. Luke, P. Kelley, F. Ngan, X. Ren, and A. Stein, 2019: Atmospheric Mercury Model Evaluation vs. Realistic Limits of Deterministic Predictions: What is Success? 14th International Conference on Mercury as a Global Pollutant, Krakow, Poland, Sept 8-13.
- Ngan, F., Christopher Loughner, and A. Stein, 2019: Evaluating the mixing characteristics in HYSPLIT with controlled tracer experiments. 23rd Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, George Mason University.
- Ngan, F., A. Stein, and Christopher Loughner, 2018: The evaluation of mixing methods in HYSPLIT using measurements from Sagebrush Tracer Experiment. 22nd Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, George Mason University.
- Ngan, F., G. Rolph and A. Stein, 2017: North America Reanalysis Data for Dispersion Applications and Recent HYSPLIT updates. U.S. Nuclear Regulatory Commission's International MELCOR Accident Consequence Code System (MACCS) User Group (IMUG) meeting, Bethesda, MD.
- Ngan, F. and A. Stein, 2017: A Long-Term WRF Meteorological Archive for Dispersion Simulations: Application to Controlled Tracer Experiments. 21st Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, George Mason University.
- Ngan, F. and A. Stein, 2016: Dispersion simulations of inline HYSPLIT for Sagebrush tracer experiment. 20th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, VA, George Mason University.

Future Plans

DATEM and Meteorological Analysis Datasets

- Major updates to the DATEM and evaluation webpages.
- The WRF dataset will be updated using the latest WRF version and new landuse data.

Western WRF Modeling Project

- Expand the forecast period to 5 days and add new graphics
- Additional comparisons of the model results with the mesonet data
- Assimilation of mesonet data into WRF to improve model performance

Tracers of Opportunity

- Build up database of areas and time periods where emissions and measurements exist and for which interferences from uncharacterized sources are minimal
- Classify by meteorological conditions, terrain type, distance from source to station
- Apply new statistical and evaluation methodologies, e.g., object-based statistics (e.g., analysis using plume features rather than fixed gridded concentration results)
- Additional meteorological and concentration measurements (ground, mobile, drones, aircraft)