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Improving emissions inputs via mobile measurements to estimate fine-scale Black Carbon concentrations through geostatistical data fusion

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Background

Transportation centers such as airports, railyards, highways, and ports are a significant source of air pollutants, pollutants associated with a myriad of adverse health outcomes. [1]

Transportation sources tend to be near other primary air pollution sources like warehouses, industrial facilities, and commercial operations.

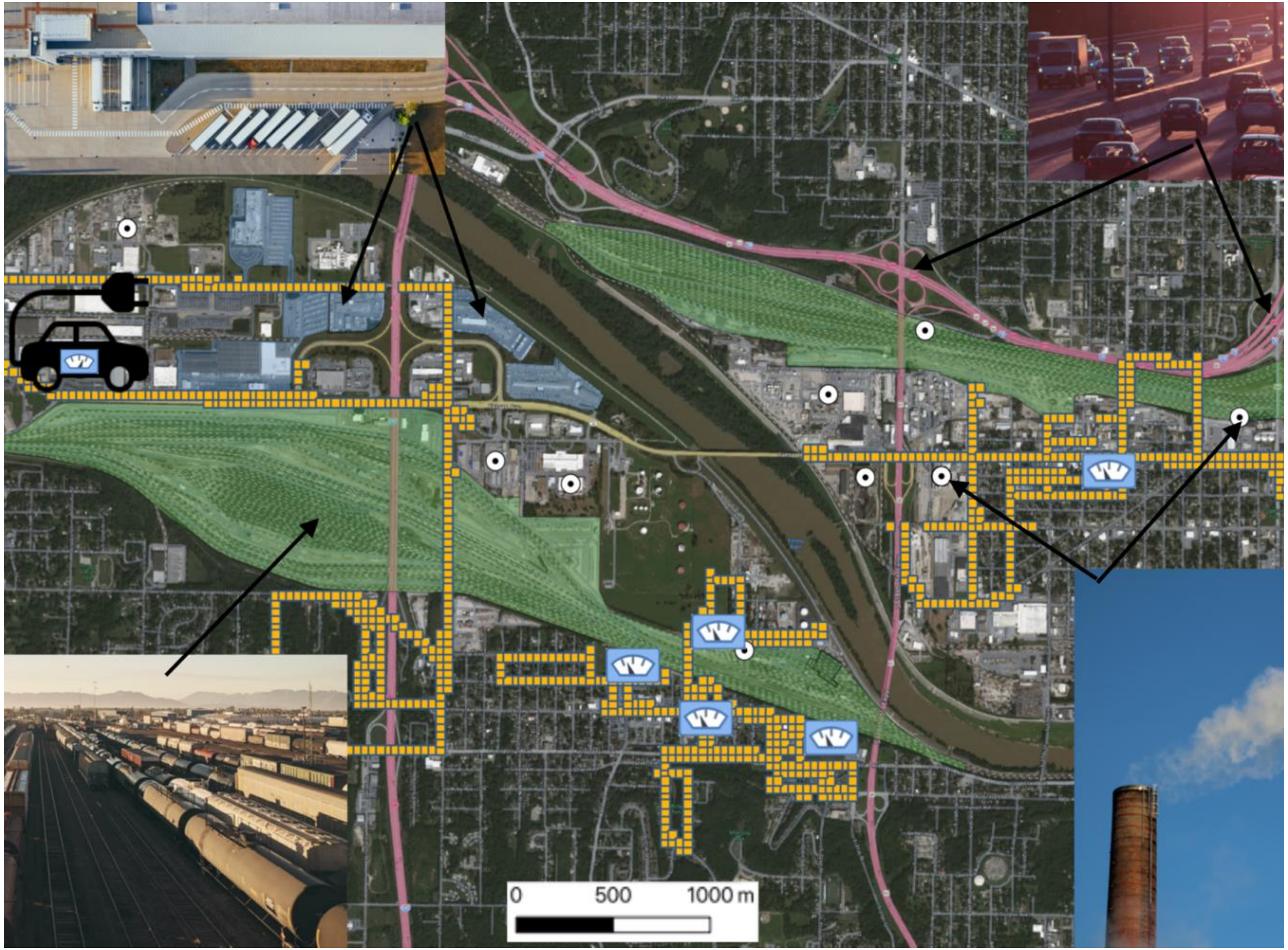
In the United States, ~45 million people reside near primary transportation sources. [2]

[1] HEI, 2010
[2] United States Census Bureau, 2007

Motivation

- Urban fine-scale characterization of air quality is vital for developing effective air pollution control strategies
- Isolating sources and quantifying their contribution is challenging in complex transportation environments[1]
  - Spatially sparse fixed observations
- Fine-scale dispersion modeling combined with fixed and mobile observations were used to characterize annual air quality and identify hot spots in Kansas City.[2]

[1]Turner et al., 2009
[2]Isakov et al., 2019



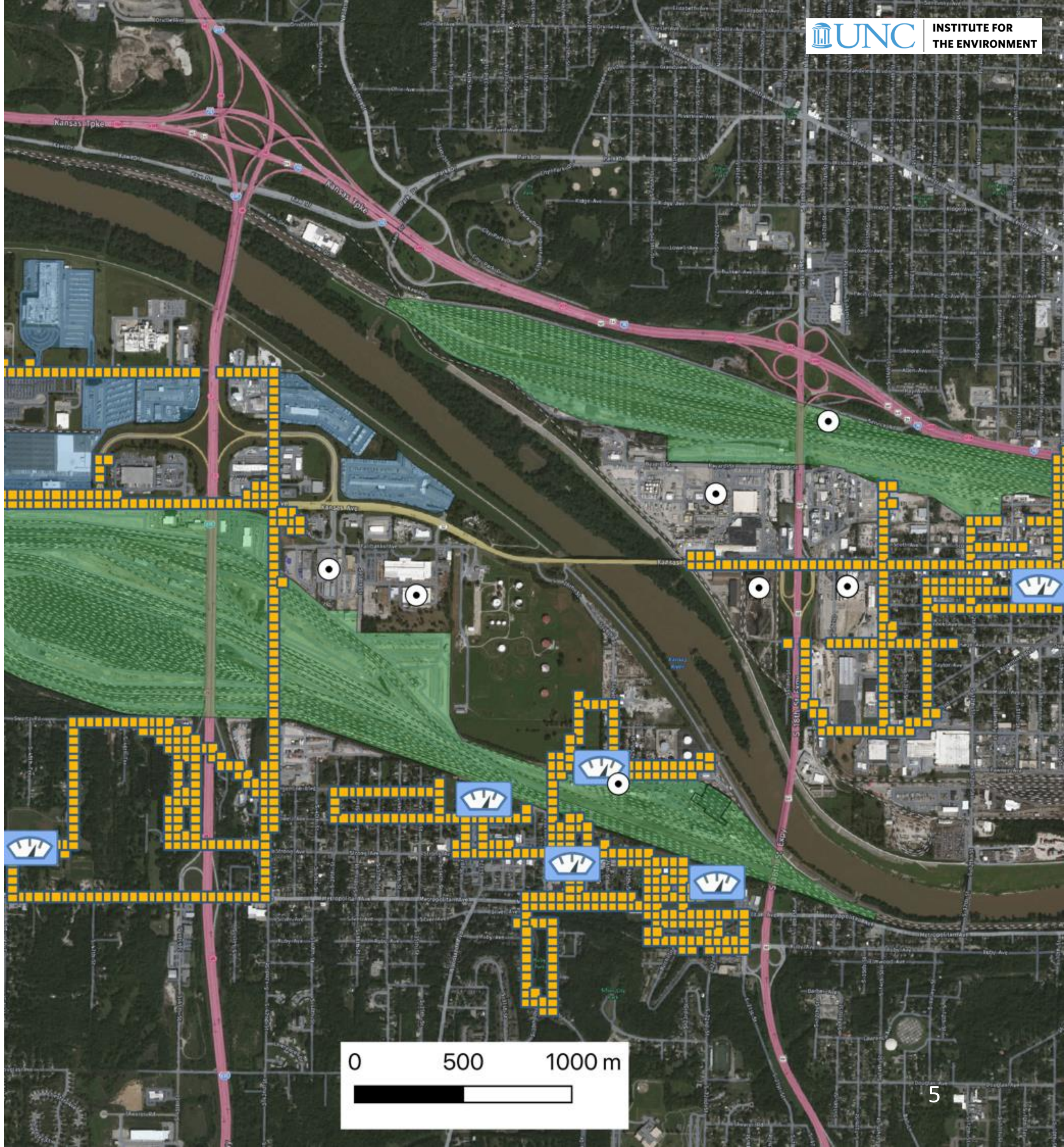
Objectives

- Expand Isakov et al., 2019 in Kansas City.
  - Increase spatial representation of mobile monitors
  - Explore finer temporal scales
  - Improve emission characterization
- Establish a method to adjust emissions and identify underrepresented sources using stationary and mobile measurements
  - Improve dispersion modeling predictions
  - Compare with unadjusted dispersion model
- Combine dispersion modeling along with stationary and mobile measurements using BME geostatistical data fusion

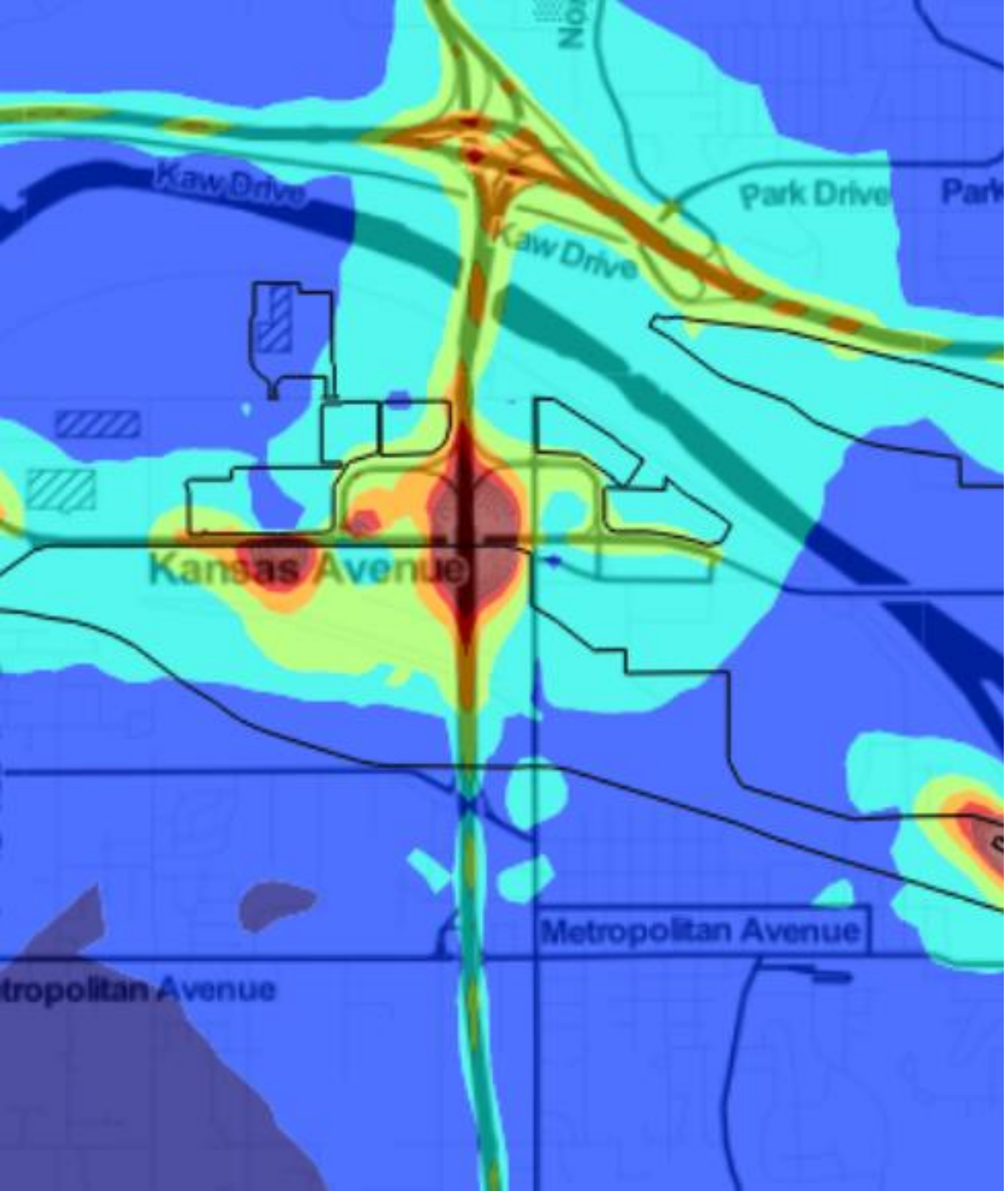
Methods
Field Campaign

Kansas City Transportation and Local-Scale Air Quality Study (KC-TRAQS) Field Campaign [1]

- October 24, 2017, to October 31, 2018
- Stationary Monitoring
  - Collected site-specific meteorological data and Black Carbon (BC) concentrations at 6 sites
- Mobile Monitoring
  - Conducted 2 mobile monitoring campaigns for 31 sampling days (Oct., Nov., Feb., & Mar.)
  - 6-10 hours of continuous sampling each day
  - Vehicle drove 15 to 20 laps along the same route
  - Gridded to 40x40 m resolution



[1]Kimbrough et al, 2019



Methods
Dispersion Model

- Utilized algorithms from the Community Air Quality Tools (C-TOOLS).[1,2]
- Input
  - Hourly meteorological observations from the Kansas City Airport
  - Isakov et al. developed local-scale emission inventory for the KC-TRAQS domain[2]
  - Background value based on the annual average from the Air Quality System (AQS) site located in Tallgrass Prairie National Preserve, Kansas
- Output
  - Hourly Black Carbon Concentrations
  - 75m by 75m grid resolution in 10km by 8km domain

[1]Isakov et al. 2017
[2]Isakov et al. 2019

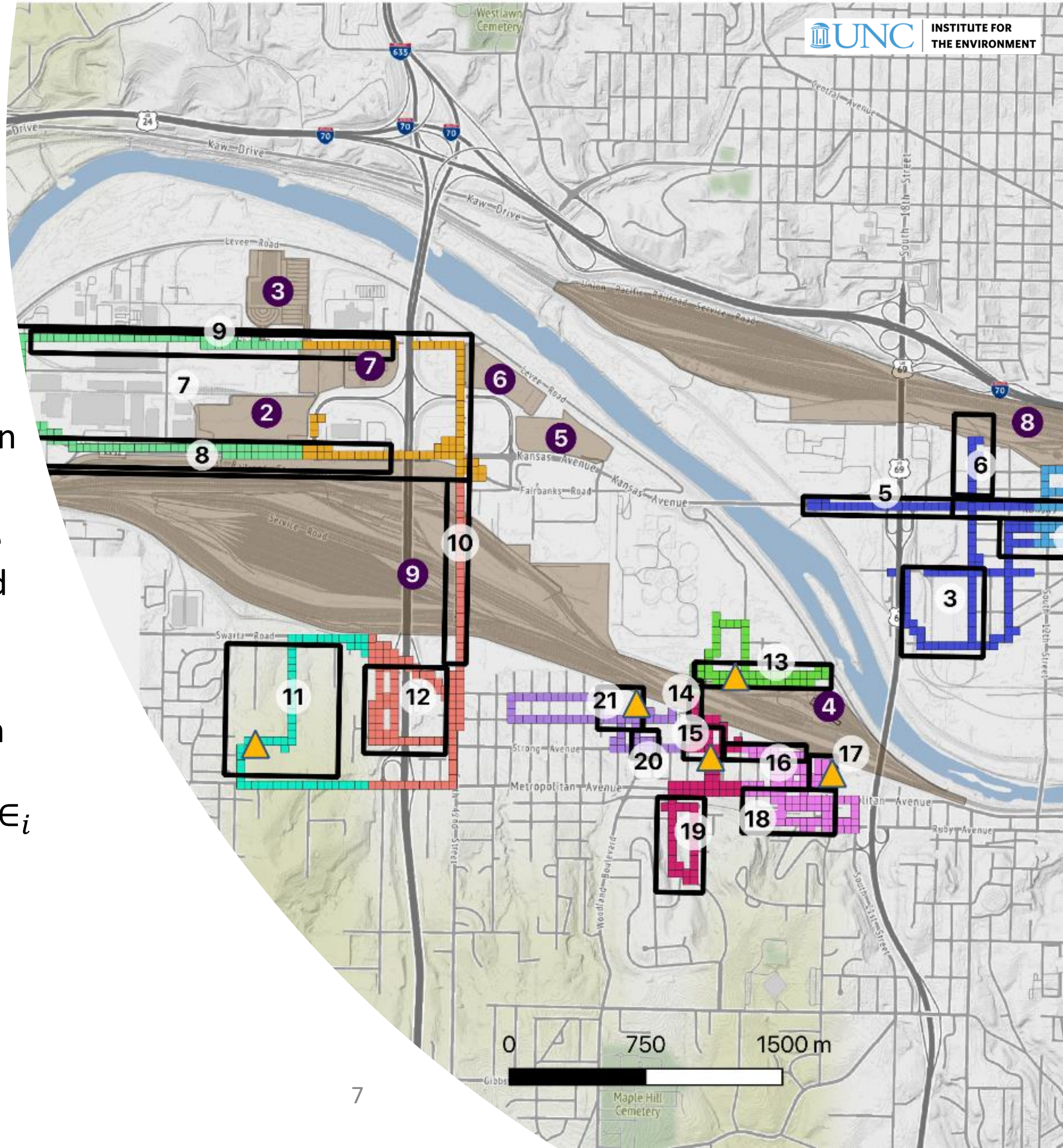
Methods

Inverse Modeling Framework

- Improve the emission characterization of our most uncertain (area) sources
- Obtain the adjustment factors by minimizing the sum of the residuals $\epsilon_i = z_{obs,i} - z_{adj,i}$, where $z_{obs,i}$ are stationary and mobile hourly observations of BC concentration at points i
- Implement in a python-based Ordinary Least Squares (OLS) regression library by defining the following linear regression equation:

$$z_{obs,i} = b_0 + b_W z_{W,i} + b_M z_{M,i} + b_{Arg} z_{Arg,i} + b_{Arm} z_{Arm,i} + \epsilon_i$$

where b_0 is the background concentration
z is the initial dispersion concentration,
b is the adjustment factor for
the Warehouses Group (W), 2 3 5 6 7
the Maintenance Facility (M), 4
the Argentine Railyard (Arg), 9
the Armourdale Railyard (Arm) 8 1



Methods
Bayesian Maximum Entropy (BME) Data fusion

X(s): Homogeneous Spatial Random Field representing the variability of ***x***

x: Residual Concentration
z: BC Concentrations
o: Offset Concentration
h: Observed locations

- 6 stationary sites
- Mobile monitoring grids

k: *gridded* unsampled locations

** Upper case represents random values and lower case represents deterministic (e.g., observed) values.*

Residual Concentration

$$x_h = z_h - o_h$$

→

***X(s)* Covariance Modeling**

Fit an exponential covariance model through the experimental covariance values obtained from x_h

↓

BME Ordinary Kriging

Estimate $\mathbf{x_k}$ by interpolating $\mathbf{x_h}$ using **BMElib** numerical library with:

- General knowledge - ***X*(*s*)** constant mean and covariance
- Site-specific knowledge - x_h treated as hard (i.e., exact) data

→

Observation Corrected Model

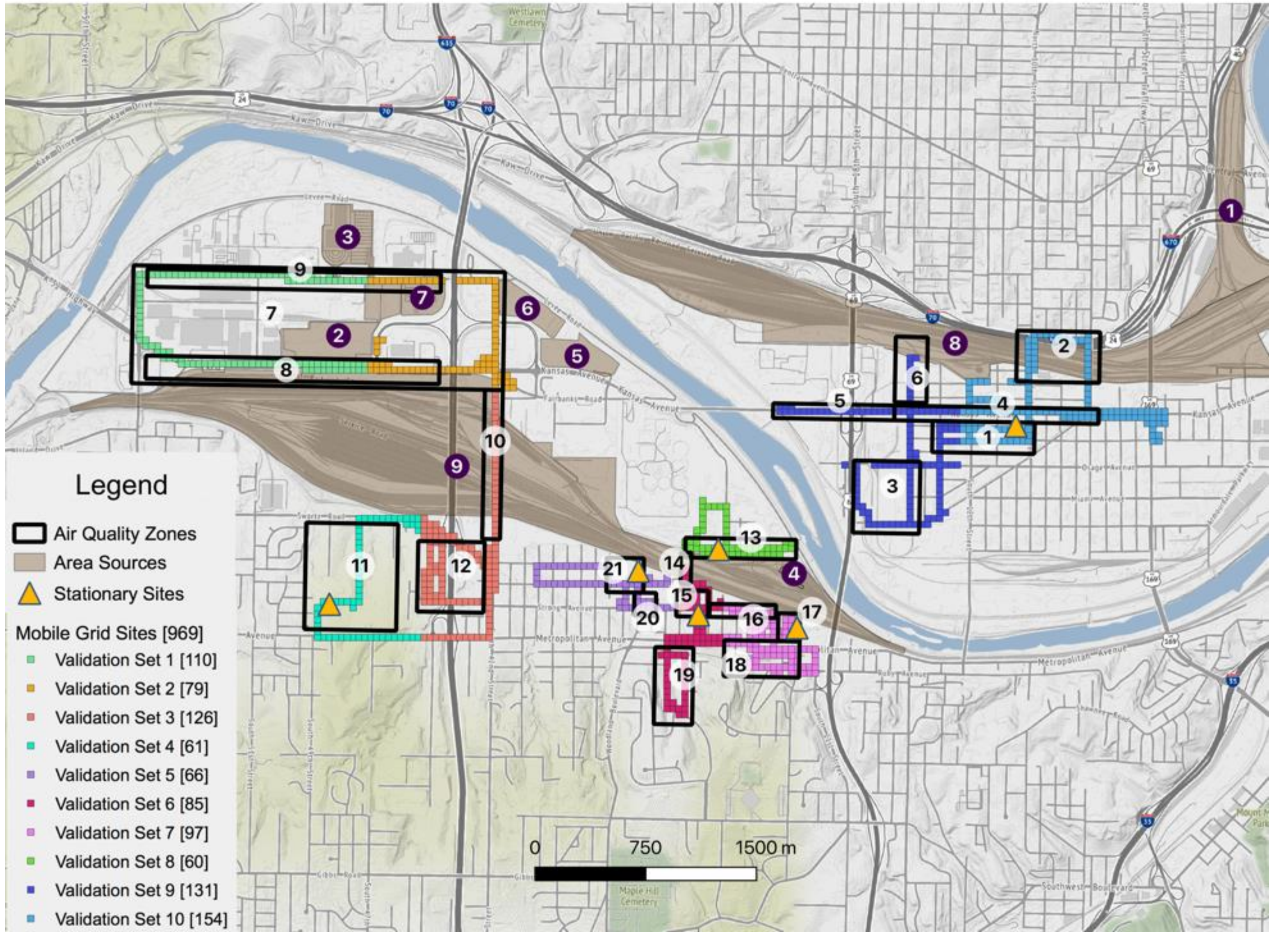
$$z_k = o_k + x_k$$

Methods
Bayesian Maximum Entropy (BME) Data fusion

- 3 Offsets defined across the space/time domain
  - **Flat BME**
    - Constant offset equal to the mean of the observations (No dispersion model)
  - **DISP BME**
    - Unadjusted dispersion model (**DISP**)
  - **I-DISP BME**
    - Adjusted dispersion model (**I-DISP**)

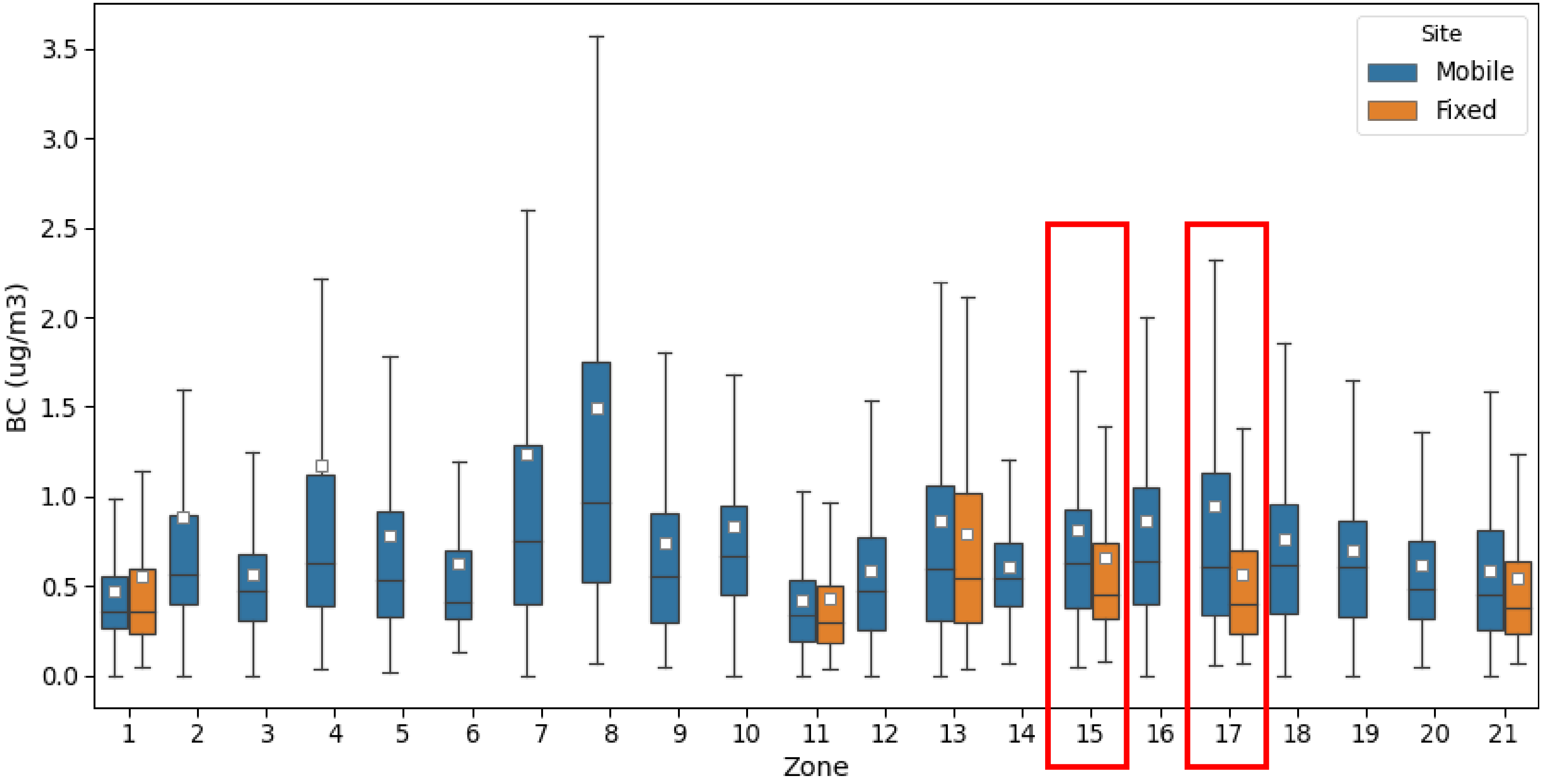
Methods
Cross-validation

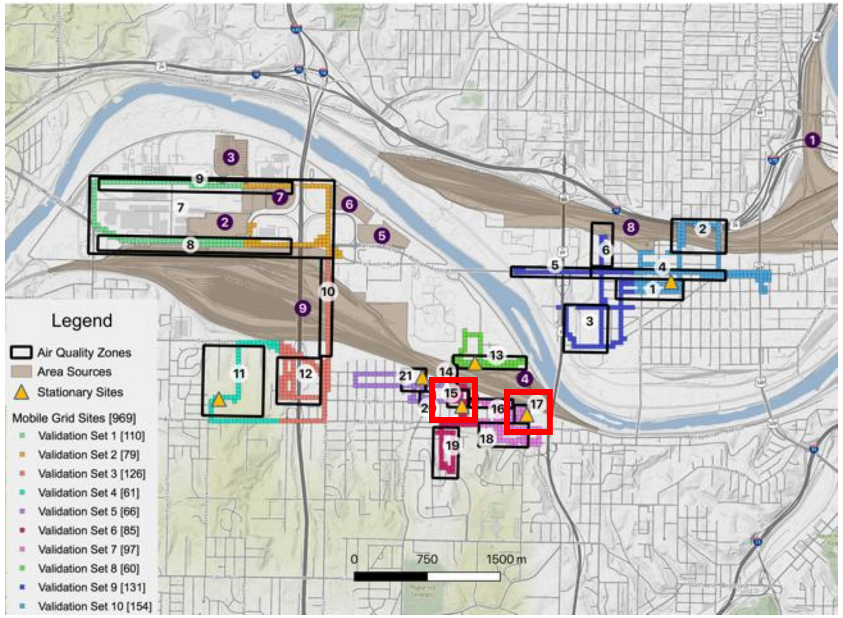
- Conventional cross-validation (conventional 10-fold)
- Spatially clustered cross-validation (clustered 10-fold)
- Spatial 2-fold cross-validation



Results
Field Campaign

Distributions of observed BC concentrations at stationary and at mobile monitoring grids for the 2017/2018 study period.





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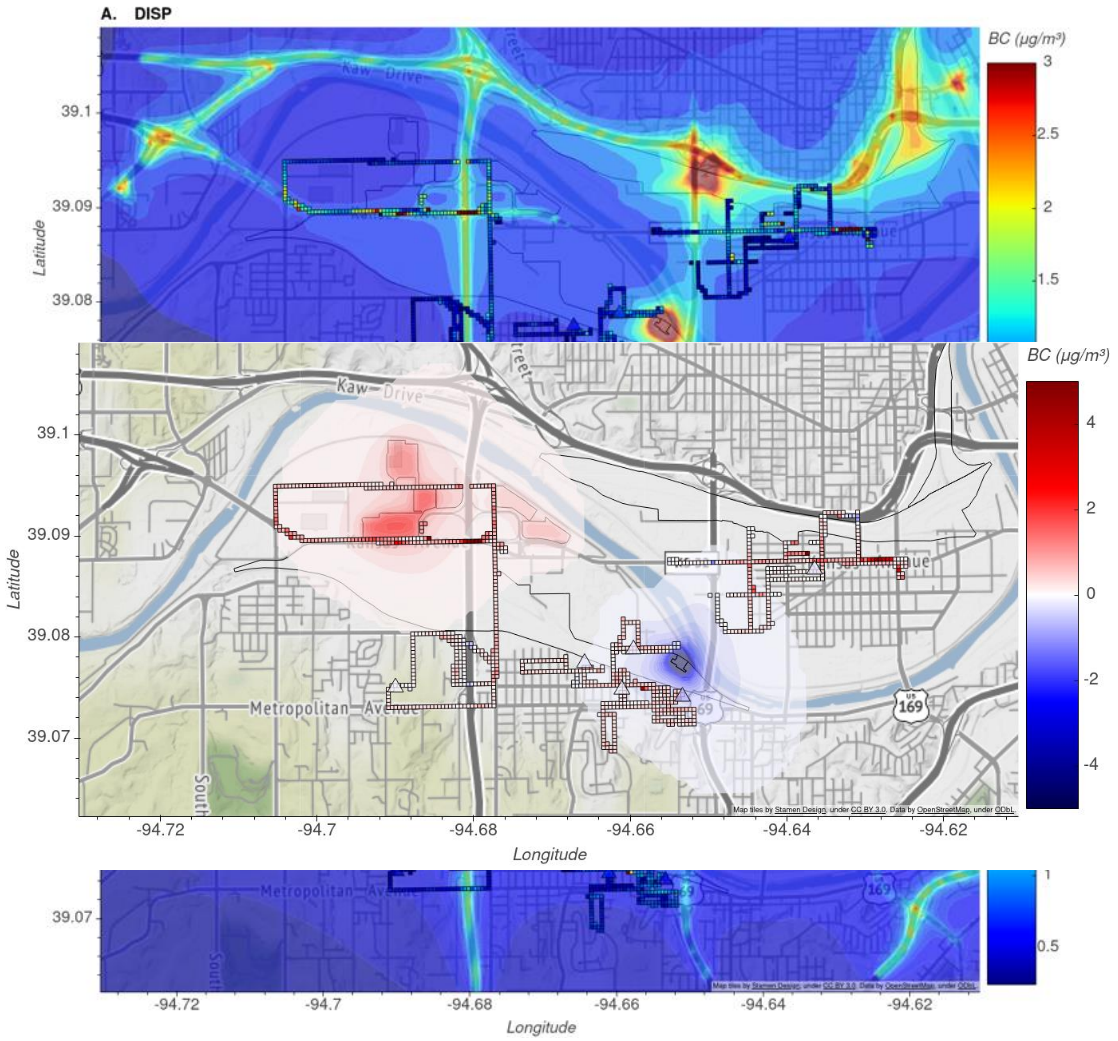
Results
Inverse Modeling

Unadjusted (DISP) and adjusted (I-DISP) area source BC emissions with adjustment factors

Area Number	Area Source	DISP Emissions (tons/year)	Adjustment Factor (95% C.I.)	I-DISP Emissions (tons/year)
1	Armstrong	0.8400	1.000	0.8400
2	Associated Wholesale Grocers	0.0032	305.8 (244.5,367.1)	0.9786
3	USPS Distribution Center	0.0012	305.8 (244.5,367.1)	0.3669
4	BNSF Maintenance Facility	1.482	0.0818 (0.0620,0.1020)	0.1186
5	UPS Freight	0.0005	305.8 (244.5,367.1)	0.1525
6	Sam’s Club Distribution	0.0004	305.8 (244.5,367.1)	0.1223
7	Estes Express Lines	0.0002	305.8 (244.5,367.1)	0.0612
8	Union Pacific Armourdale Yard	0.4670	1.000	0.4670
9	Santa Fe Argentine Yard	1.542	0.9187 (0.841,0.996)	1.417

Annual BC Concentrations

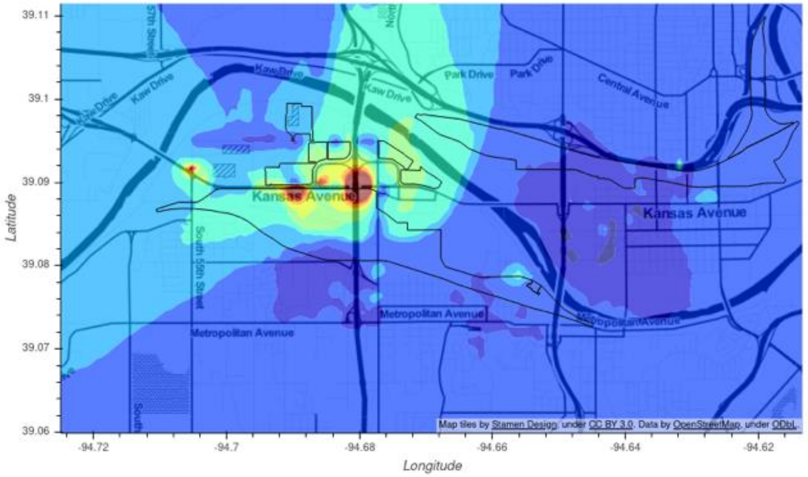


Overall, these adjustments in emissions contribute to a 4% increase of the total area source emissions.

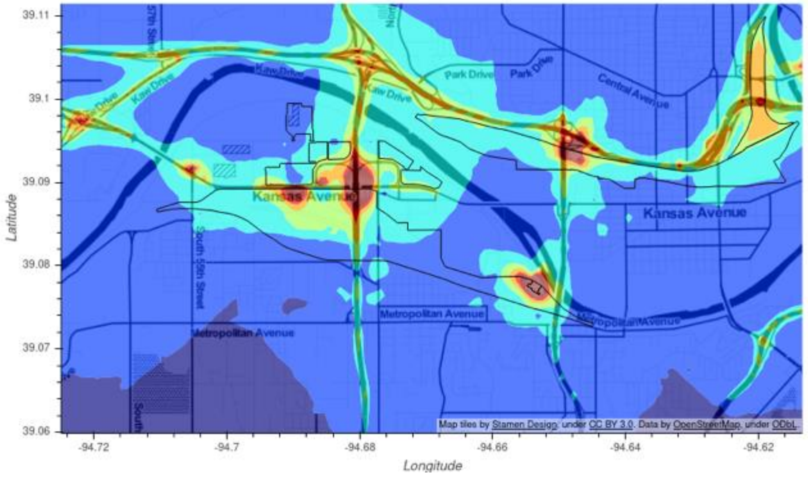
Results
BME Data Fusion

Monthly Average BC (ug/m^3) for October 2017

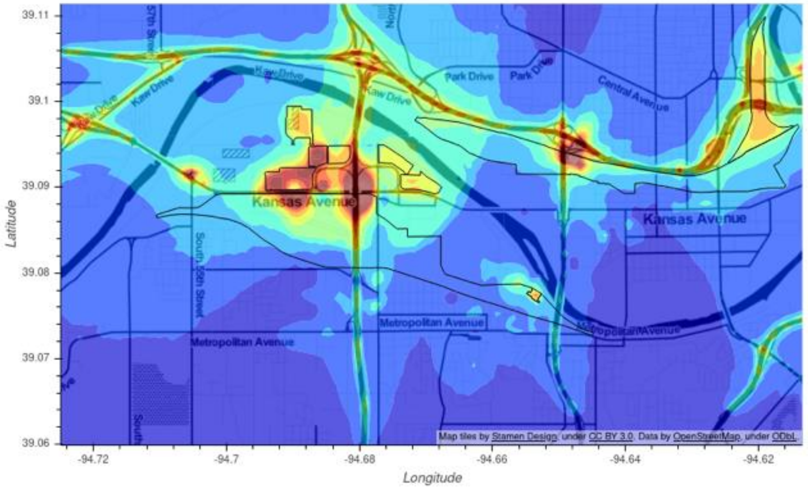
Flat BME



DISP BME



I-DISP BME

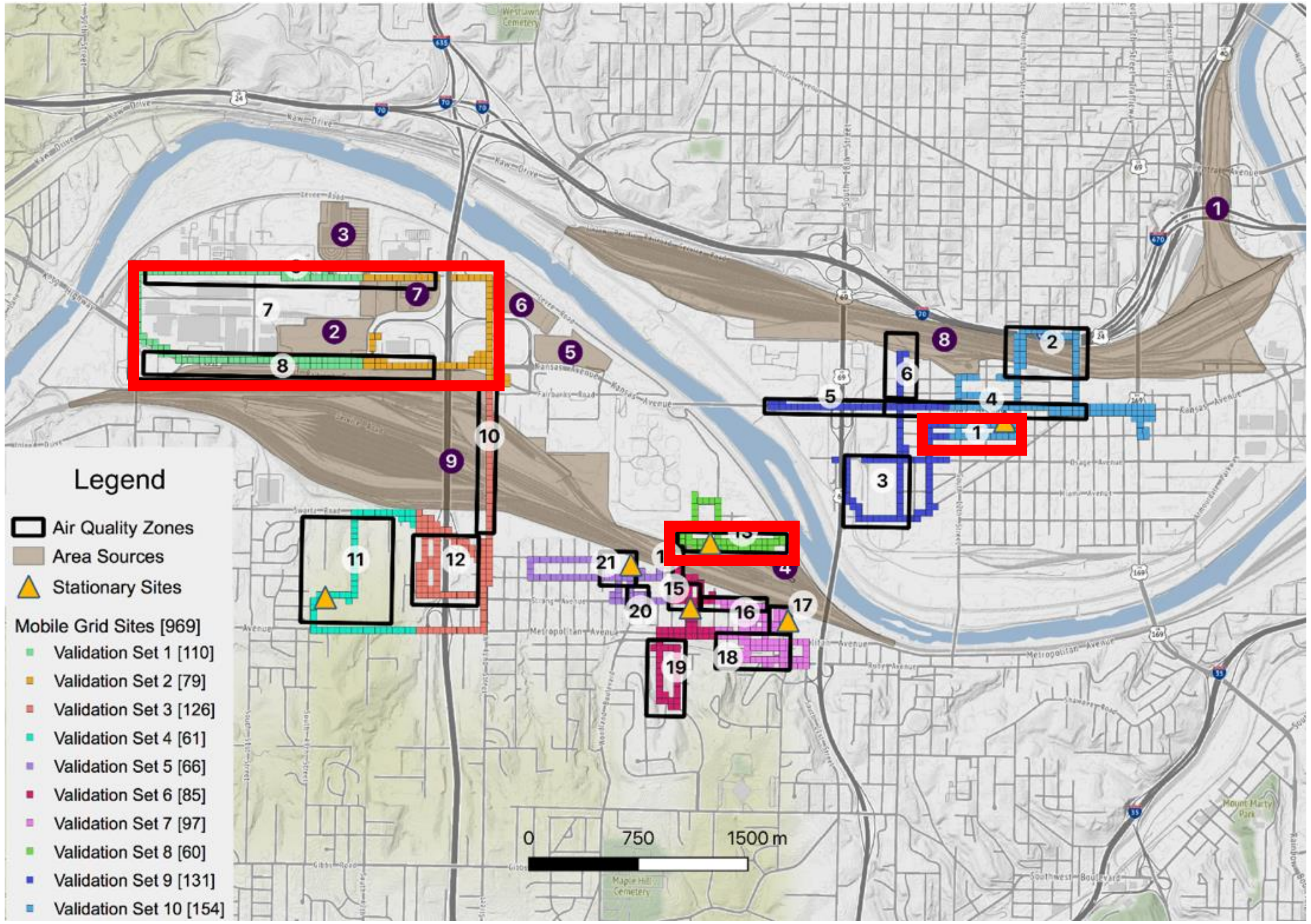


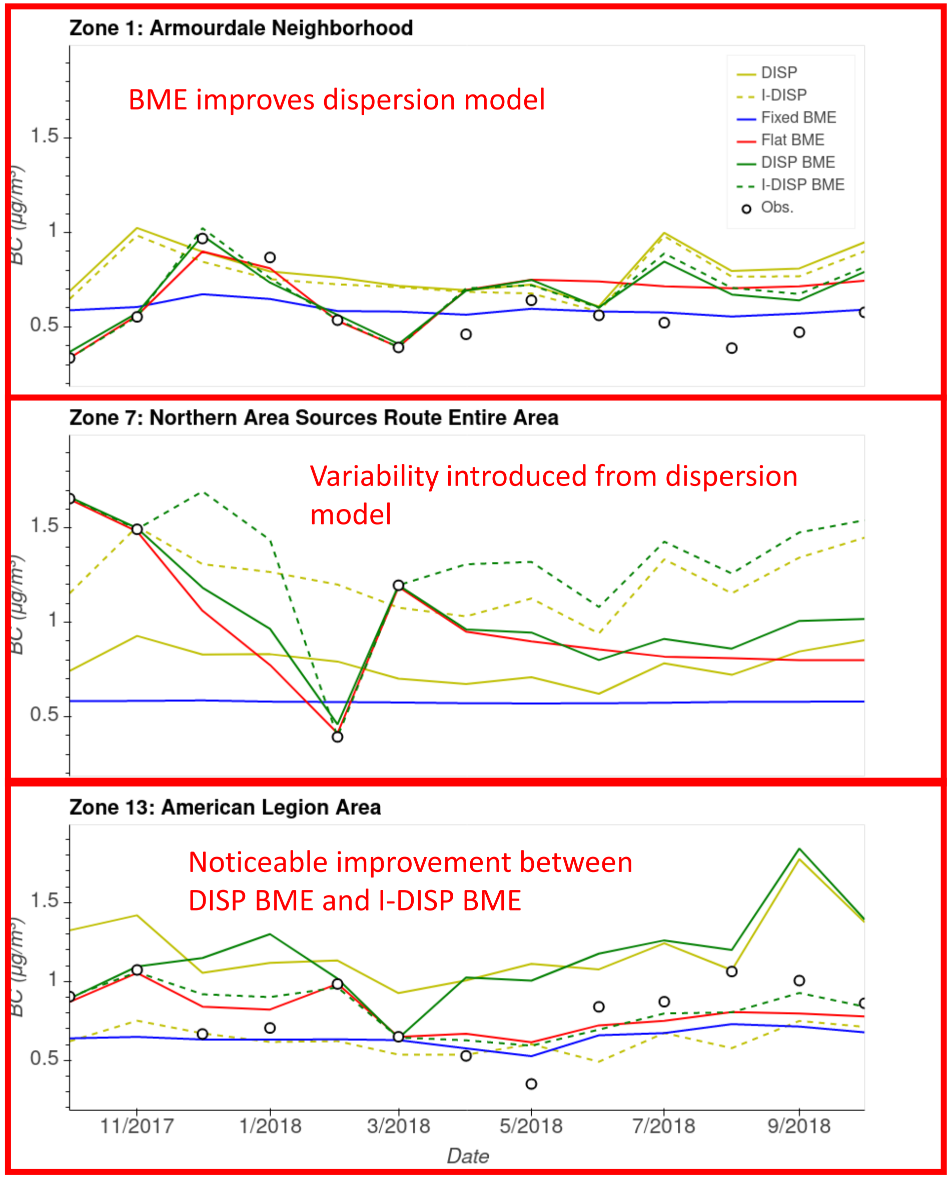
Flat BME lacks elevated concentrations gradients in the vicinity of roadways and railyards.

The main differences between DISP and I-DISP are depicted in the vicinity of the warehouses and the maintenance facility.

Results

BME Data Fusion





Results

Cross-Validation

R^2 for Cross-Validation Techniques for Monthly Averages.						
	DISP (R^2)	I-DISP (R^2)	Cross-Validation Method	Flat BME (R^2)	DISP BME (R^2)	I-DISP BME (R^2)
BC Monthly Average	0.070	0.109	2-Fold	0.001	0.063	0.092
			Clustered 10-Fold	0.107	0.150	0.169
			Conventional 10-Fold	0.798	0.786	0.787

Emission adjustments improved R^2 values by up to 56% from DISP to I-DIPS.

2-fold cross-validation shows an increase of a factor of 90 for I-DISP when compared to Flat.

10-fold conventional cross-validation shows that all BME methods have a R^2 of ~0.80.

Conclusion

- Used a combination of dispersion modeling, fixed and mobile measurements from KC-TRAQS with data fusion methods to characterize air quality
- Applied emissions adjustments through Inverse Modeling
  - Improved emissions inputs for dispersion modeling applications
- Applied BME data fusion to create monthly spatial maps of air pollutant concentrations
  - Identify hot spots in the study area
  - Identify contributions from local air pollution sources
- Cross-validation analysis shows model performance improvement when applying inverse modeling and BME data fusion

Future Work

- Address non-Gaussian uncertainty associated with measurements taken from mobile monitors due to temporal sparsity
  - Use BME soft data capability to assign uncertainty to mobile measurements
- Address non-Gaussian uncertainty associated with the dispersion model
  - Use the Constant Air quality Model Performance (CAMP) approach to account for the non-linear and non-homoscedastic behavior of the model
- Implement BME data fusion at time scales finer than monthly concentration averages

Acknowledgment

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References

- HEI. *Traffic-Related Air Pollution: A Critical Review of the Literature on Emissions, Exposure, and Health Effects.*; 2010.
- U.S. Census Bureau. American Housing Survey for the United States : 2007. *Curr. Hous. Reports* 2007.
- Isakov, V.; Arunachalam, S.; Baldauf, R.; Breen, M.; Deshmukh, P.; Hawkins, A.; Kimbrough, S.; Krabbe, S.; Naess, B.; Serre, M.; Valencia, A. Combining Dispersion Modeling and Monitoring Data for Community-Scale Air Quality Characterization. *Atmosphere (Basel).* **2019**, *10* (10), 610. https://doi.org/10.3390/atmos10100610.
- Isakov, V.; Barzyk, T.; Arunachalam, S.; Naess, B.; Seppanen, C.; Monteiro, A.; Sorte, S. Web-Based Air Quality Screening Tool for near-Port Assessments: Example of Application in Porto, Portugal. In *HARMO 2017 - 18th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Proceedings*; Hungarian Meteorological Service, 2017; Vol. 2017-Octob, pp 258–262. https://doi.org/10.1016/j.envsoft.2017.09.004.
- Kimbrough, S.; Krabbe, S.; Baldauf, R.; Barzyk, T.; Brown, M.; Brown, S.; Croghan, C.; Davis, M.; Deshmukh, P.; Duvall, R.; Feinberg, S.; Isakov, V.; Logan, R.; McArthur, T.; Shields, A. The Kansas City Transportation and Local-Scale Air Quality Study (KC-TRAQS): Integration of Low-Cost Sensors and Reference Grade Monitoring in a Complex Metropolitan Area. Part 1: Overview of the Project. *Chemosensors* **2019**, *7* (2), 26. https://doi.org/10.3390/chemosensors7020026.