The University of Texas at Austin
McKetta Department of Chemical Engineering
Cockrell School of Engineering

HEI energy

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HEI Energy Study Webinar

Predictive, source-oriented modeling and measurements to evaluate community exposures to air pollutants and noise from unconventional oil and gas development

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UT Austin Team

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Measurements
Stakeholder Engagement
Modeling

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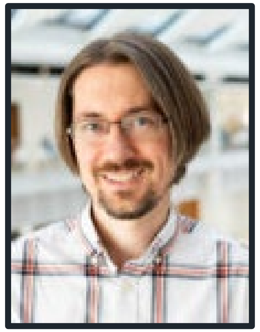

Measurements

David Allen
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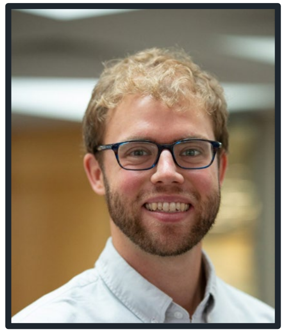
Modeling
Stakeholder engagement

Lucas Henneman
George Mason U.



Exposure modeling

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Public Health

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Biostatistics

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UT Austin Project Overview

Main goal : to generate a broadly applicable community model which can assess exposures to air pollutants from UOGD and inform future health studies

→ TRACER (TRAcking Community Exposures and Releases) model

Model combines fine-scale spatial-temporal **emission models**, molecular fingerprints of emission sources, and **dispersion modeling**

Targeted field measurements, in part to evaluate and refine the model

Evaluate exposures, inform future health studies

Initial focus on **Eagle Ford Shale**. Project was expanded to include modeling in the **Marcellus Shale** and measurements in the **Permian**

Focus in today's presentation

1. Estimating emissions from UOGD
2. Coupling emissions with dispersion models
3. Coupling emissions with chemical transport models
4. Applying the modeling framework to production regions

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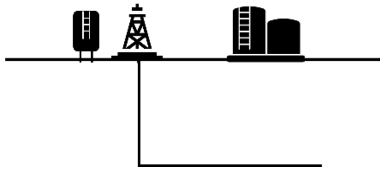
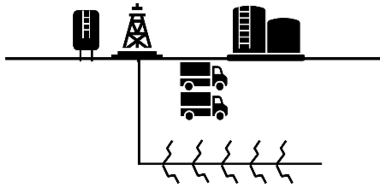
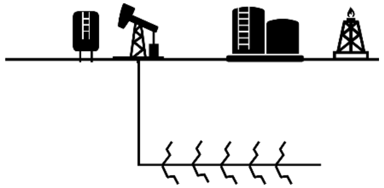
Key features needed in an emissions model

- High spatial and temporal resolution
- Estimate emissions for multiple chemical species
- Characterize differences in emission compositions for different sources
- User-friendly methods and tools

Sources modeled

- For each source, detailed calculation procedures developed:
  - Temporal and spatial allocation information
  - Speciation profiles

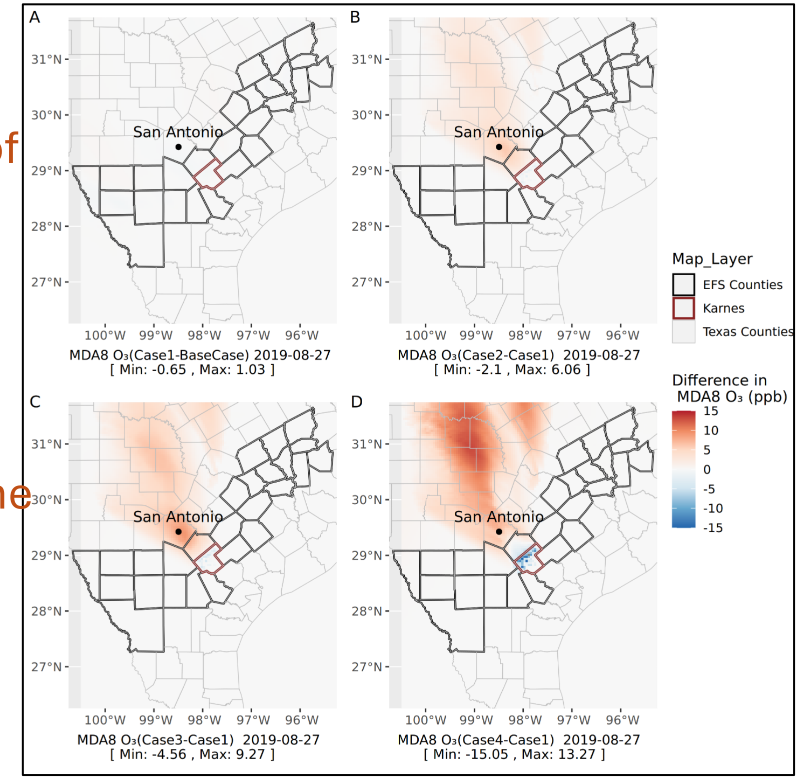
Drilling	Completion/Hydraulic Fracturing	Production
		
Well site primary sources: 1. Drilling Rigs 2. Mud Degassing 3. Fugitive Emissions	Well site primary sources: 4. Hydraulic Fracturing Pumps 5. Well Completion Venting 6. Fugitive Emissions	Well site primary sources: 7. Artificial Lift Engines 8. Associated Gas Venting 9. Condensate Tanks 10. Crude Oil Tanks 11. Dehydrators 12. Fugitive Emissions 13. Gas-Actuated Pneumatic Pumps 14. Heaters 15. Compressor Engines 16. Liquids Unloading 17. Pneumatic Controllers 18. Produced Water Tanks 19. Flaring Gathering and Boosting site primary sources 20. Compressor Engines 21. Compressor blowdowns 22. Compressor start-ups 23. Dehydrators 24. Acid Gas Removal

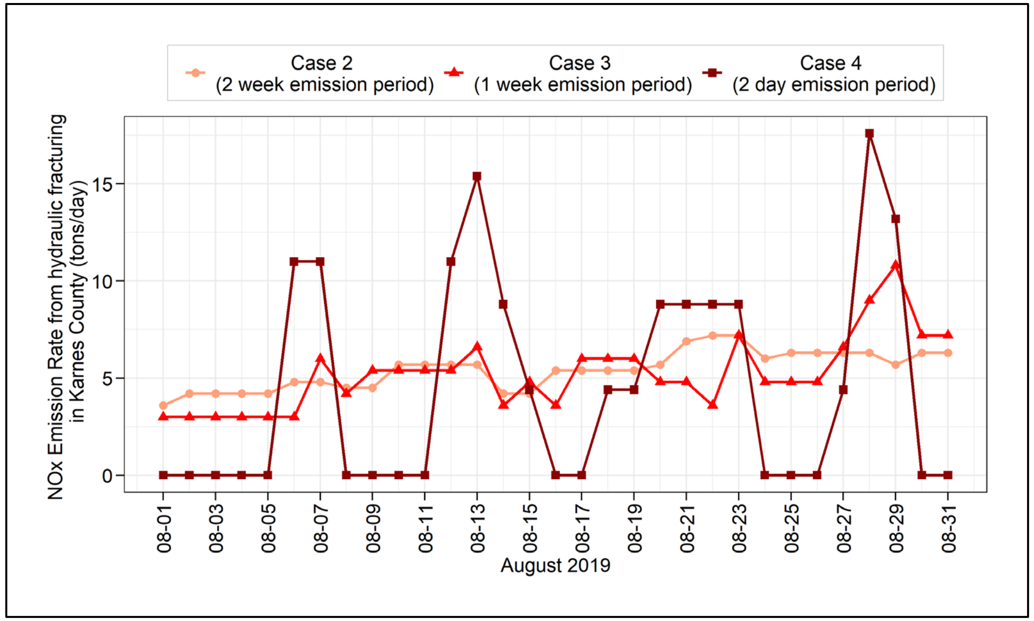
Case study of importance of spatial and temporal allocation: NOx emissions from hydraulic fracturing

- One of the largest NOx emission sources in oil and gas production regions
- Contribution of this work is spatial and temporal allocation of emissions
  - Typical allocations are county level, annual average emissions
  - Allocation by sources location and time of fracturing does not change annual total emissions but can change localized, hourly emission rates by 3 orders of magnitude
  - Potential implications for regional ozone formation

Spatial allocation leads to predictions of ozone hot spots →

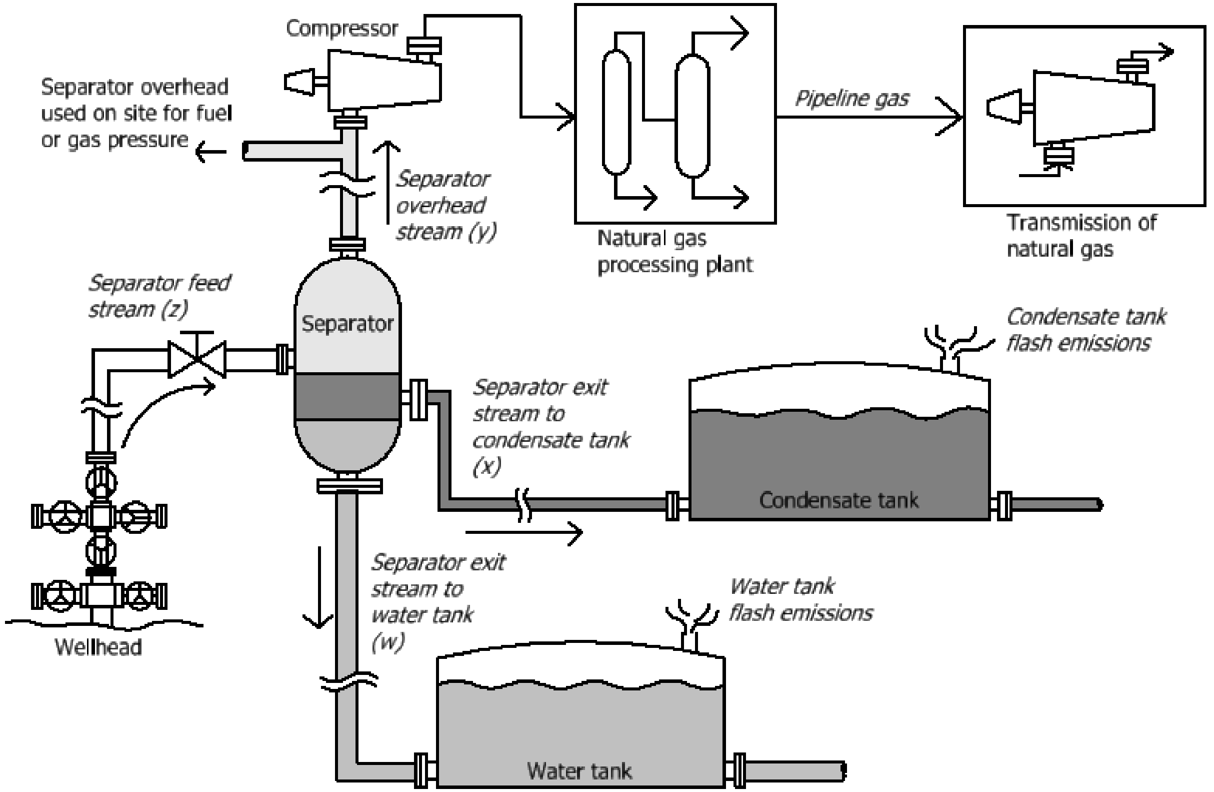
Temporal allocation leads to changes in the magnitude of the predicted ozone hot spots





Estimating speciation for production sources

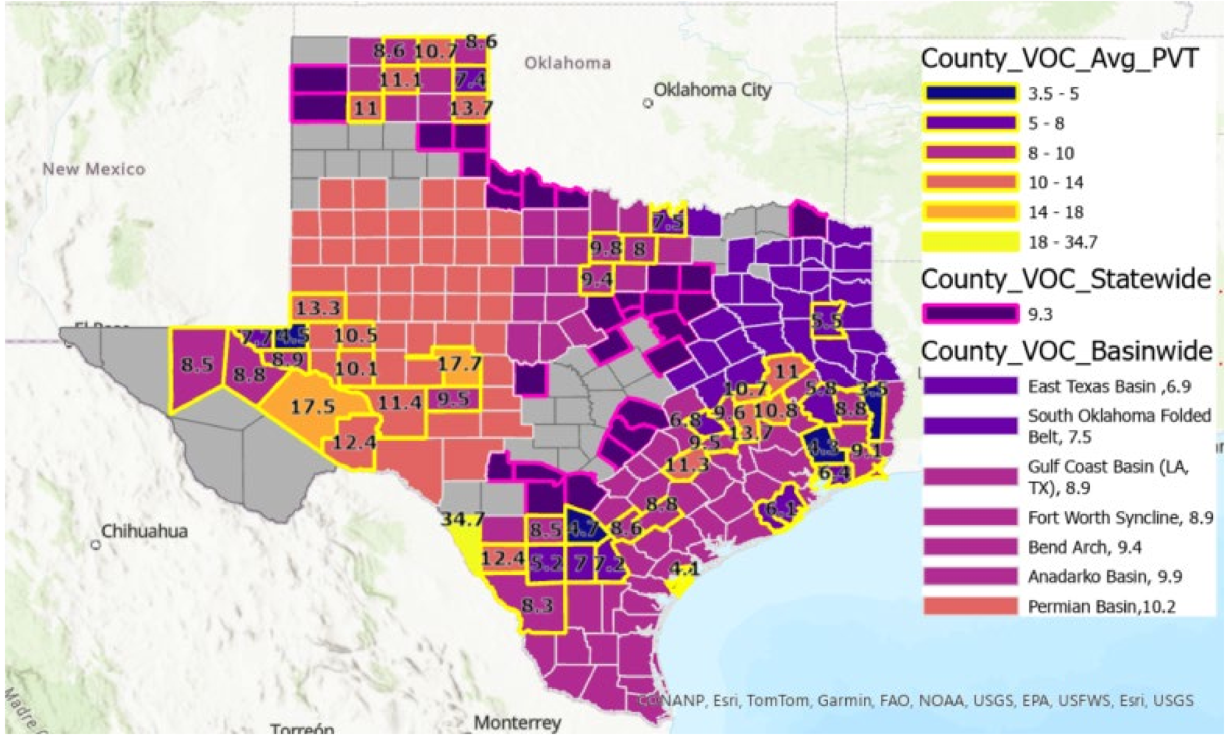
- Significant differences in emission compositions by source
- For any given source, emissions data can vary from site to site due to differences in operations and differences in geology
- Limited public data on speciation
- Develop speciation datasets
- Extend previously developed emission composition tool to include key species such as BTEX



Compile stream composition databases

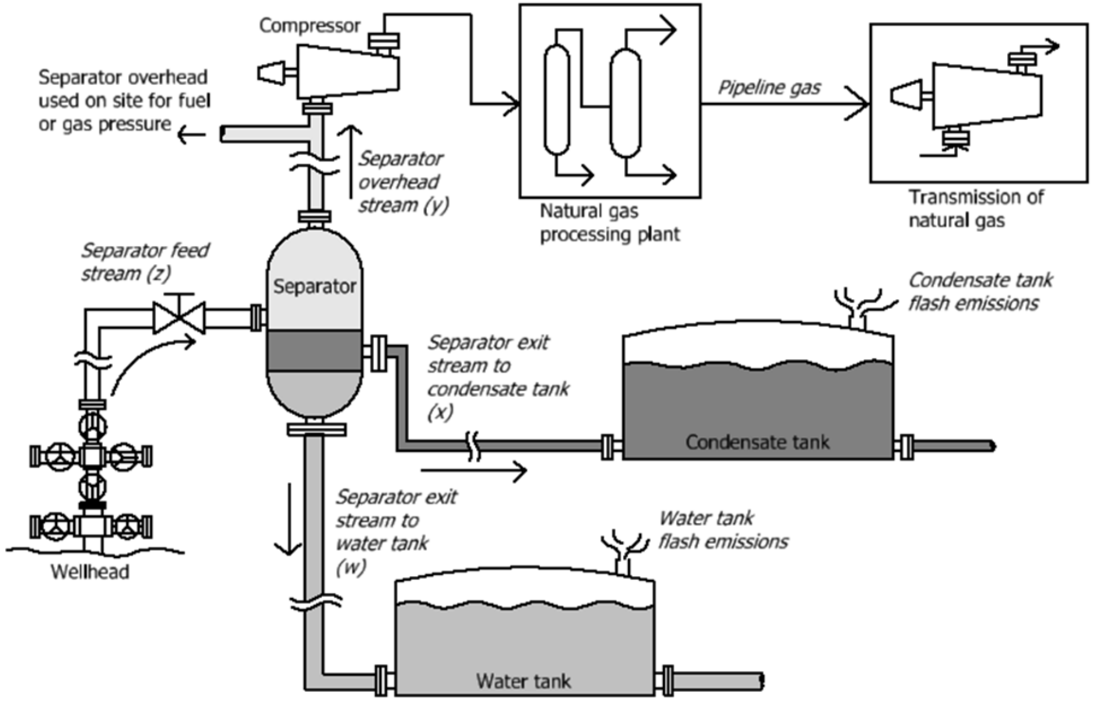
Case study: Produced gas compositions in Texas

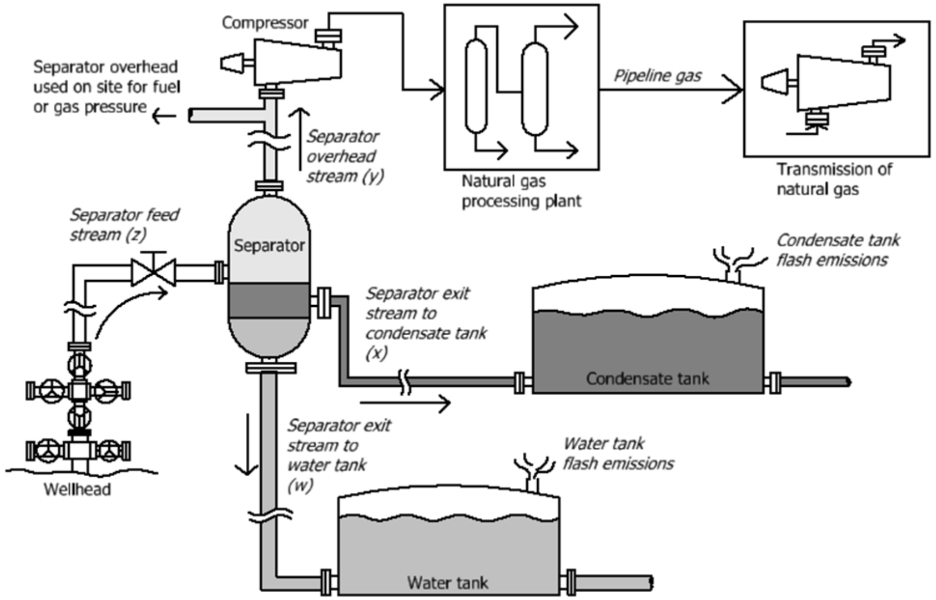
- County level produced gas composition data
- Speciated profiles as well as total VOC estimates
- Based on hundreds of publicly accessible "PVT" reports

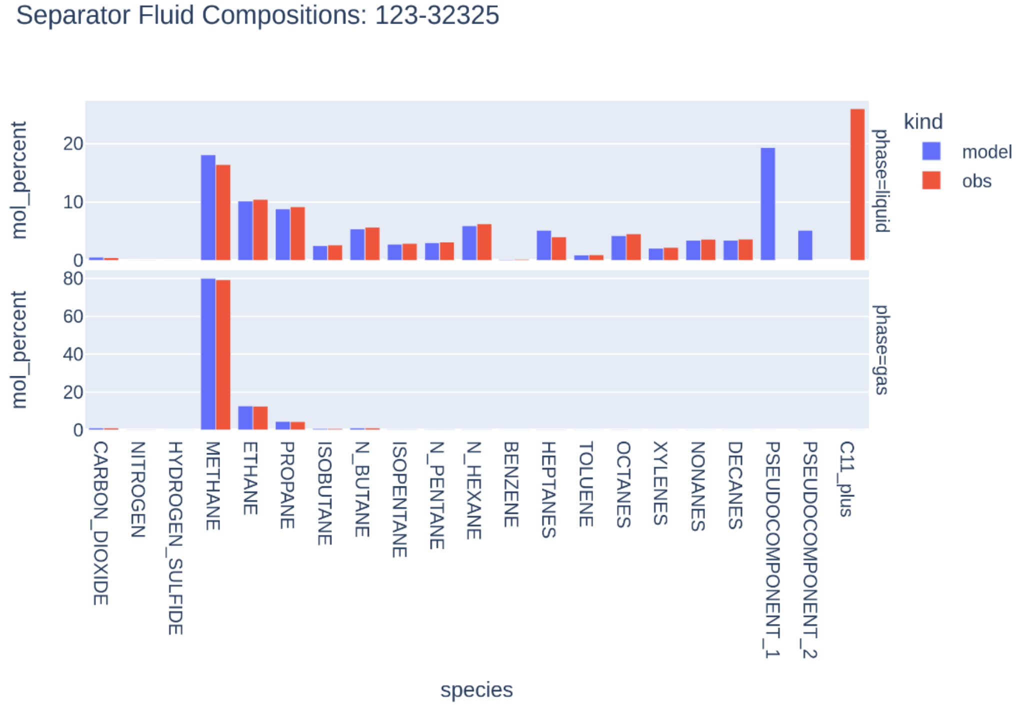


Estimating speciation for select air toxics (Case study of BTEX)

- Previous work developed searchable database of tank flash compositions tied to produced gas compositions
- Previous work only speciated light alkanes; model extended to predict BTEX and heavier alkanes
- Analyses done for Eagle Ford; speciations are likely to be basin specific; data for other basins being developed







- For a limited number of cases in the Eagle Ford, both hydrocarbon liquid and gas phase compositions were available for the separator, including BTEX compounds and alkanes through C10
- Thermodynamic model expanded to include these species
- Modeled and reported compositions compared to assess model performance
- Thousands of simulations performed for varying separator temperatures and pressures
- Speciation profiles developed for Eagle Ford production region

Speciation profiles for emission sources

Source	**Speciation profile**
Well site and tank batteries	
Drilling engines	EPA oil and gas tool
Mud degassing	Study specific speciation profile
Hydraulic fracturing pumps	EPA oil and gas tool
Completion flowbacks	Study specific speciation profile
Artificial lift engines	EPA oil and gas tool
Associated gas venting	Study specific produced gas composition by county
Condensate/crude tank venting	Study specific oil tank vent composition by county
Produced water tank venting	Study specific vent tank vent composition by county
Fugitives (leaks)	Study specific produced gas composition by county
Pneumatic pumps	Study specific produced gas composition by county
Pneumatic controllers	Study specific produced gas composition by county
Heaters	EPA oil and gas tool
Liquid unloadings	Study specific produced gas composition by county
Flares	Study specific speciation profile
Gathering and boosting sites	
Compressor engines	EPA oil and gas tool
Dehydrators	Study specific produced gas composition by county
Acid Gas Removal	Study specific produced gas composition by county
Flares	Study specific speciation profile
Gas processing plants	
Site total emissions	EPA oil and gas tool
Flares	Study specific speciation profile
Transmission facilities	
Site total emissions	EPA oil and gas tool

Key findings

- UOGD emission sources have complex spatial and temporal distributions that can impact exposures
- UOGD emission sources have can highly variable compositions that impact exposures
- Source by source calculation methods have been developed for estimating emissions, their spatial distributions and temporal distributions
- Speciation profiles have been developed based on data collected by the HEI study team and based on publicly available data and thermodynamic/process simulation analyses

Focus in today's presentation

1. Estimating emissions from UOGD
2. Coupling emissions with dispersion models
3. Coupling emissions with chemical transport models
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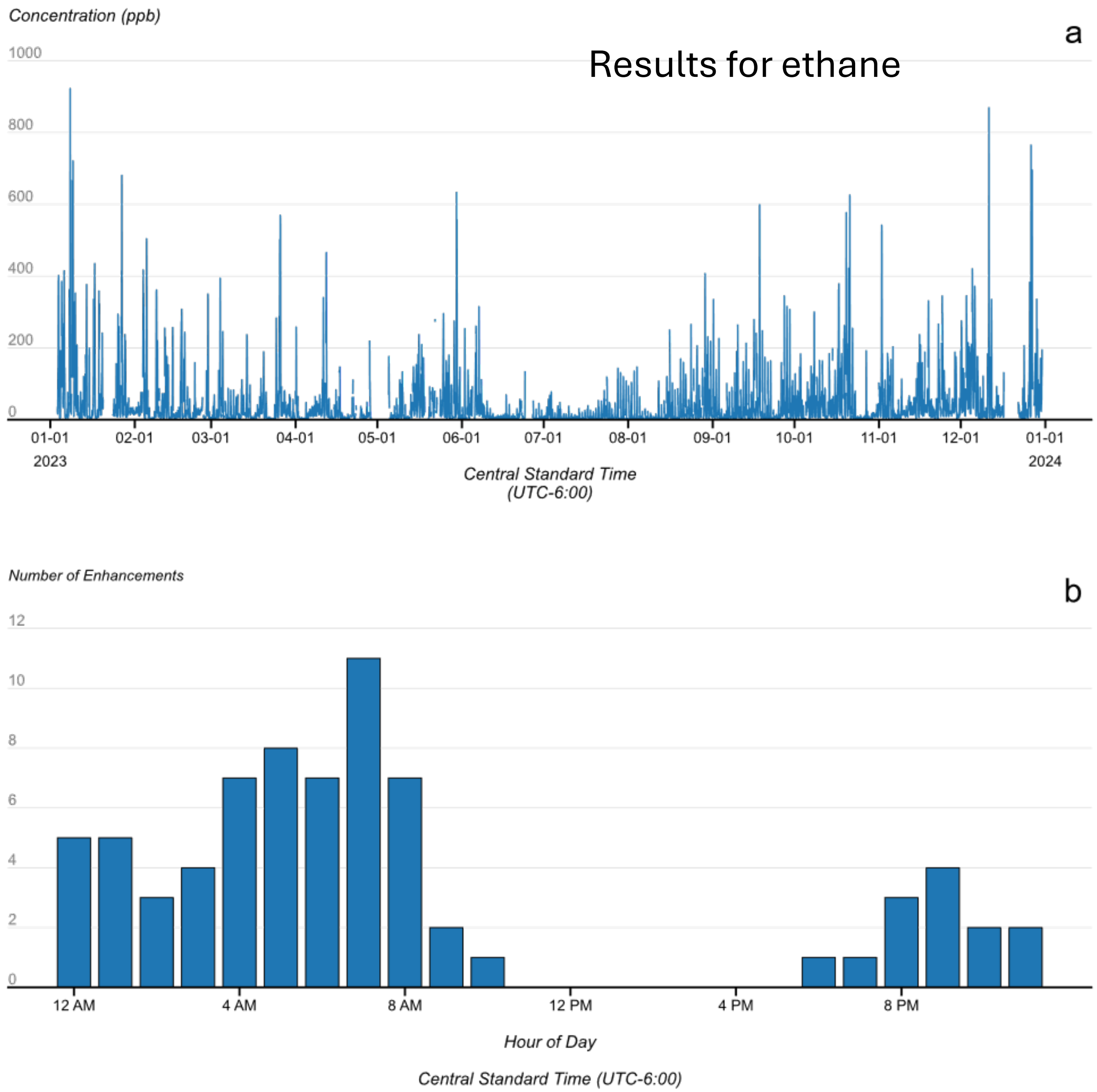
Accurately represent a concentration time series at an off-pad receptor point in an UOGD production region

- Year-long time series of hourly averaged hydrocarbon concentrations at a receptor site in the Eagle Ford Shale oil and gas production region (Karnes City, Texas)
- Highly variable observed concentrations, with short duration peak concentrations observed at night
- Same phenomena observed in other regions (e.g., Permian)
- Same phenomena observed for other species (e.g., heavier alkanes, benzene)

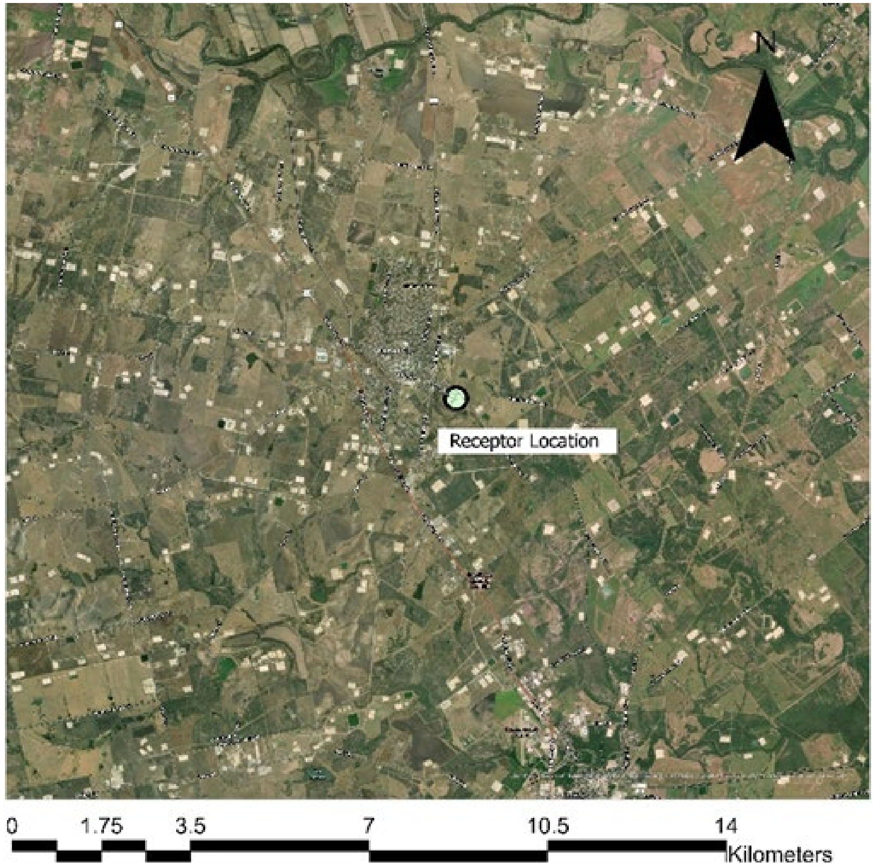


Potential causes of elevated concentrations at night

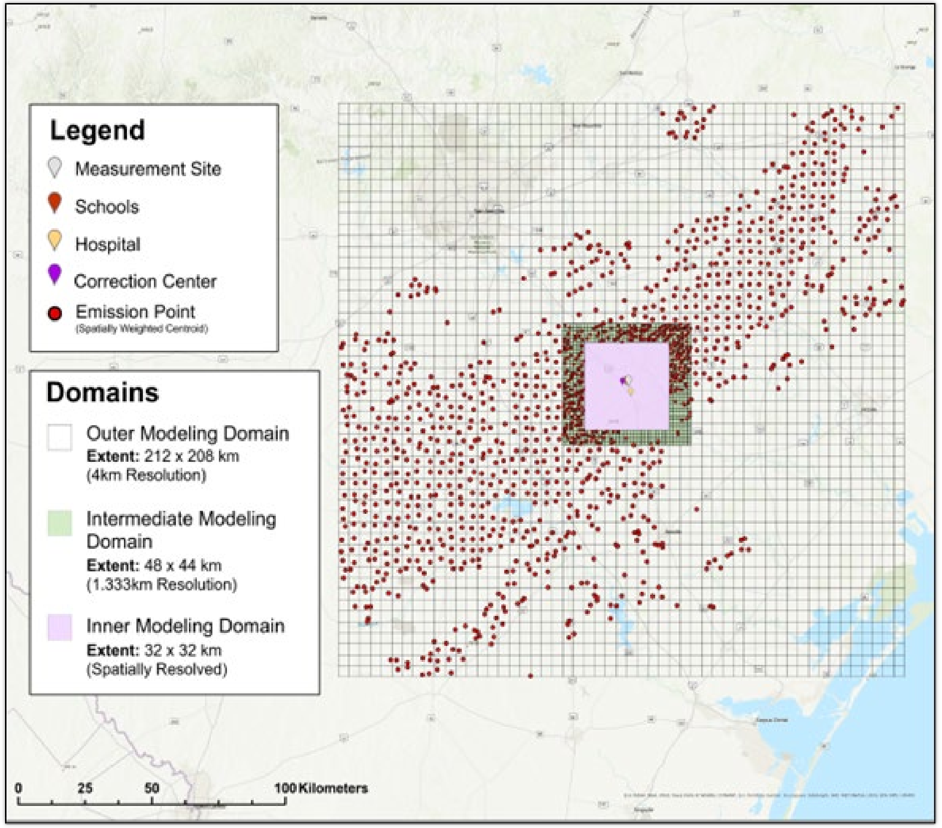
- Regional collapse of the boundary layer; not consistent, as the sole cause, with observations
  - Monitors located with ~20 km of each other all have peak concentrations at night but days and times of peak concentrations vary
  - Normalizing concentrations using boundary layer height is not an effective predictor
- Routine emissions coupled with low night-time wind speeds and low night-time mixing heights
  - Modeled using emissions model and gaussian-puff dispersion model (Calpuff)
- Non-routine emission events
  - Events detected, potential source locations and frequencies determined by identifying observations not accounted for by routine emissions

A large domain is required for dispersion modeling

Satellite image of region



Nested modeling domain extends over 200 km by 200 km region

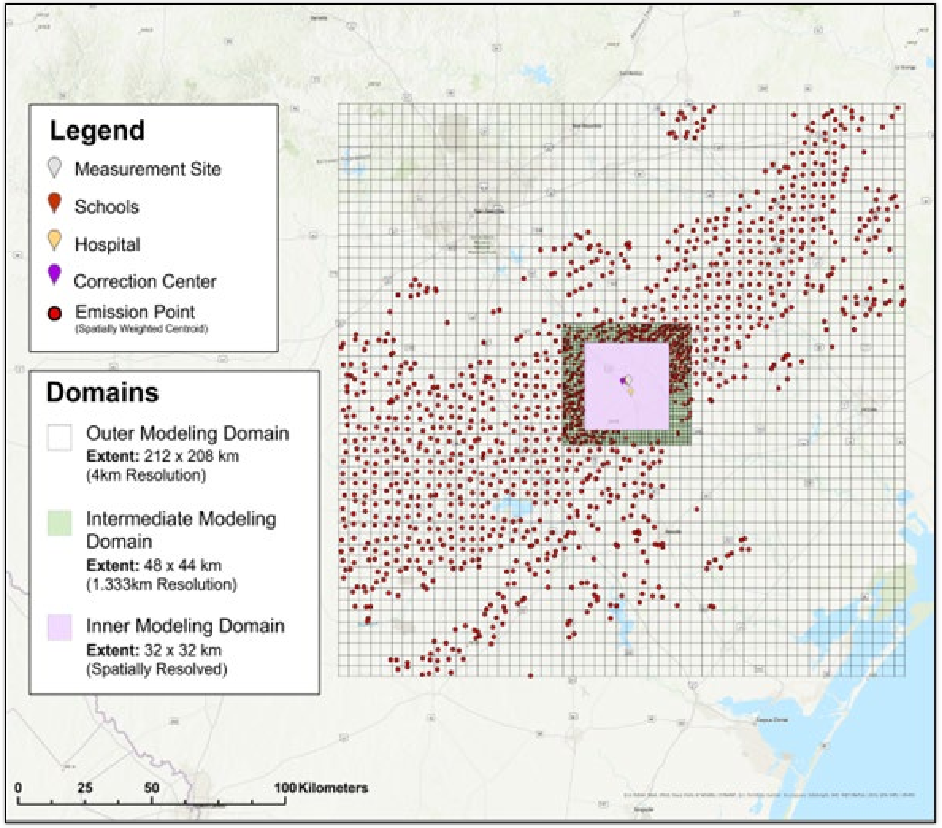


A large domain is required for dispersion modeling

Fractions of mean observed concentration due to sources within 100 km of receptor point

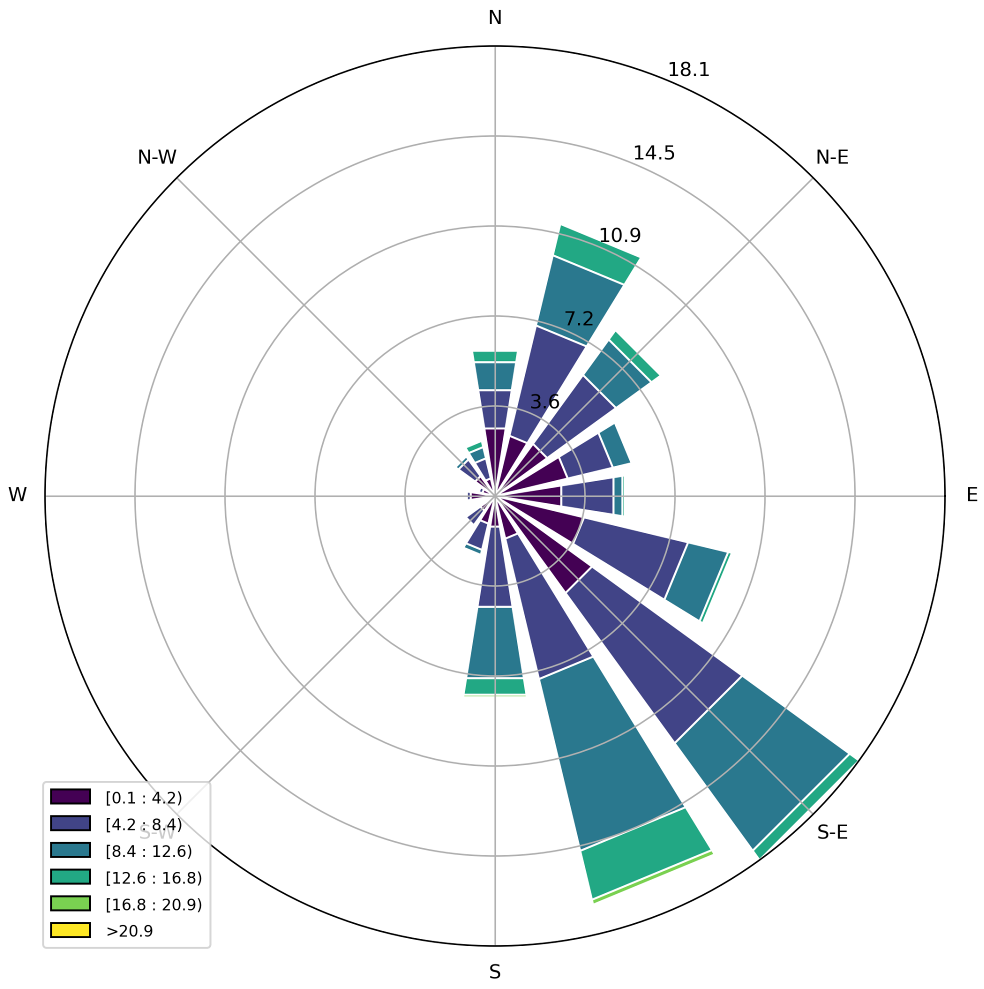
- Sources within 5 km: 38% of mean value accounted for
- Sources within 10 km: 67% of mean value accounted for
- Sources within 20 km: 88% of mean value accounted for
- Sources within 50 km: 98% of mean value accounted for
- These results are specific to the Eagle Ford; similar work underway in the Permian

Nested modeling domain extends over 200 km by 200 km region



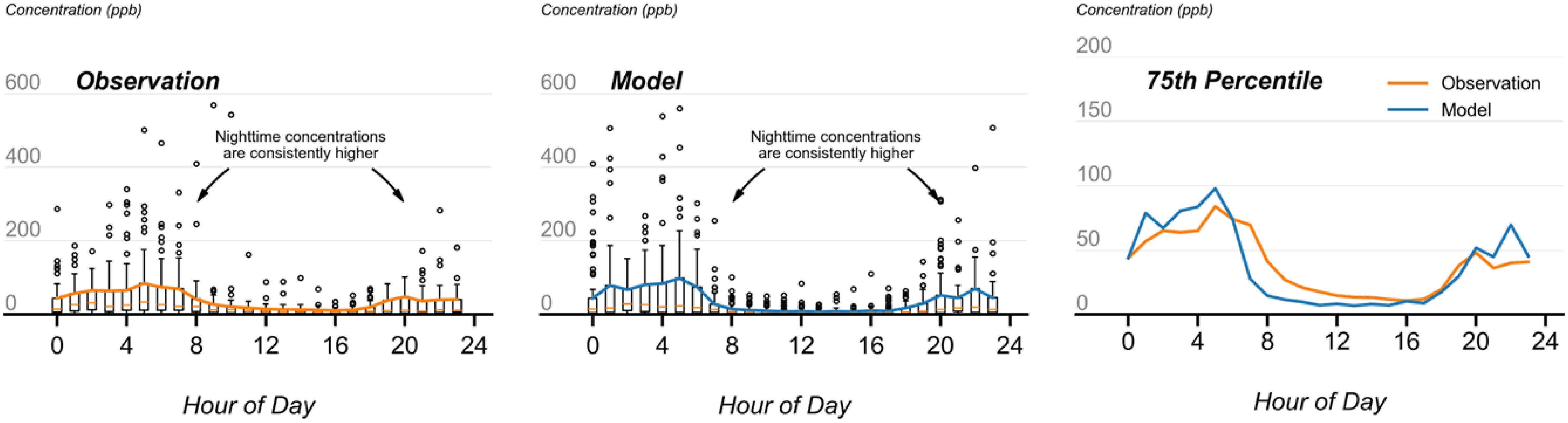
Dispersion modeling

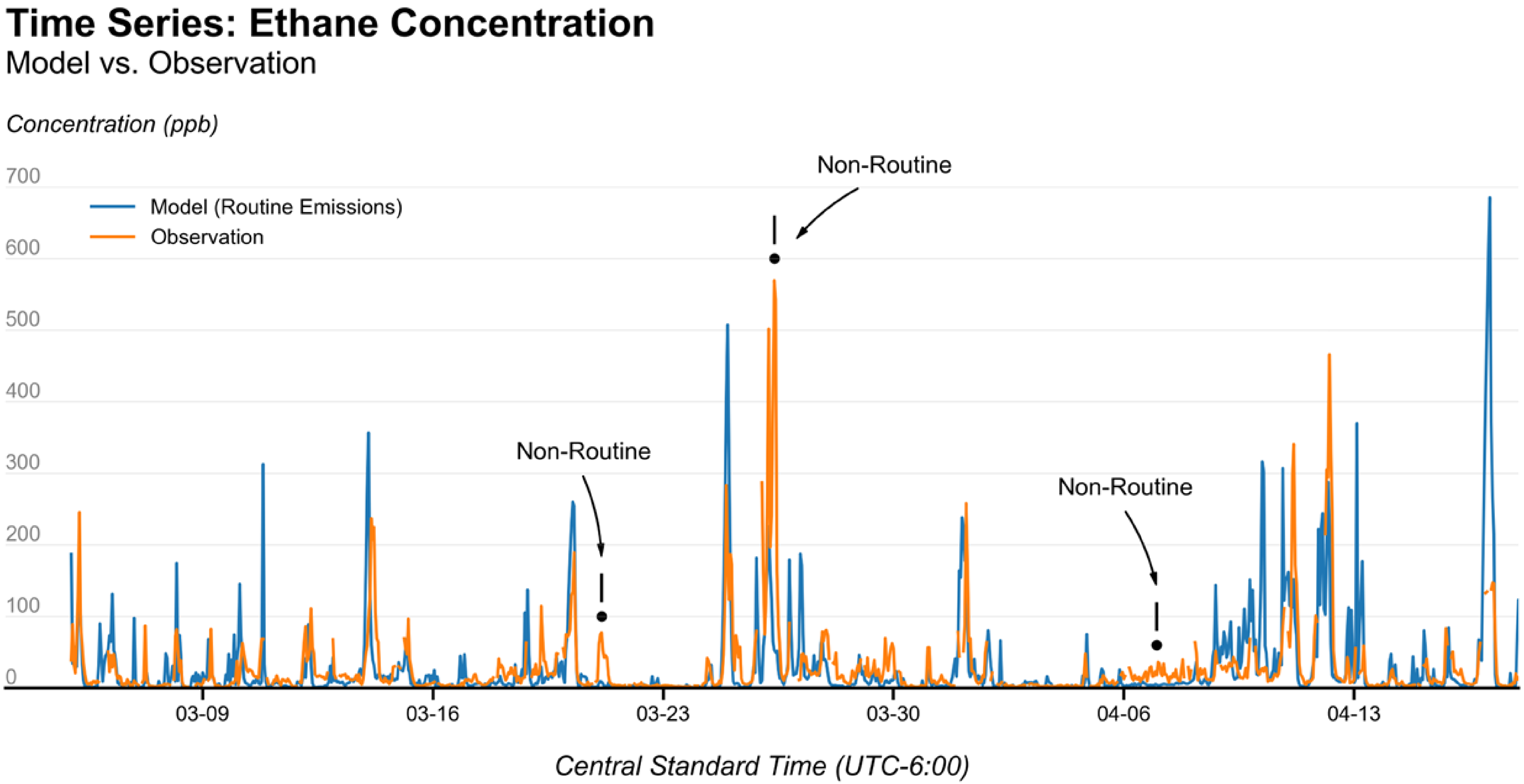
- 82 day period, March
- CALPUFF v7.2, CALMET v6.5 with 4 km horizontal spatial resolution and 10 vertical layers at a 1-hour time resolution
- Multiple local meteorological data sources (HRRR modeling, 5 minute wind speeds at receptor sites, >20 additional stations)

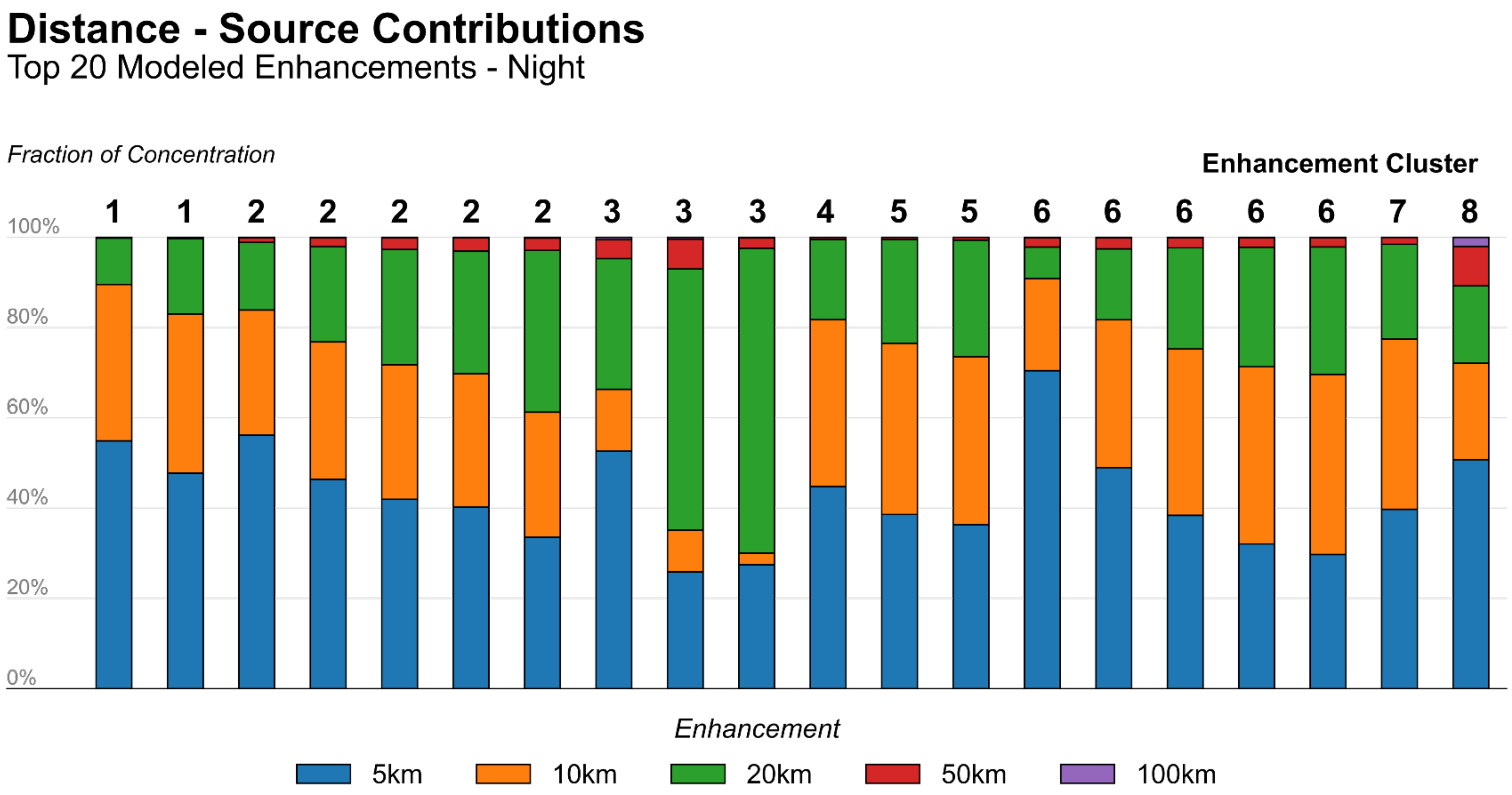


Time-of-Day Distributions of Concentration Enhancements

Model Vs. Observation

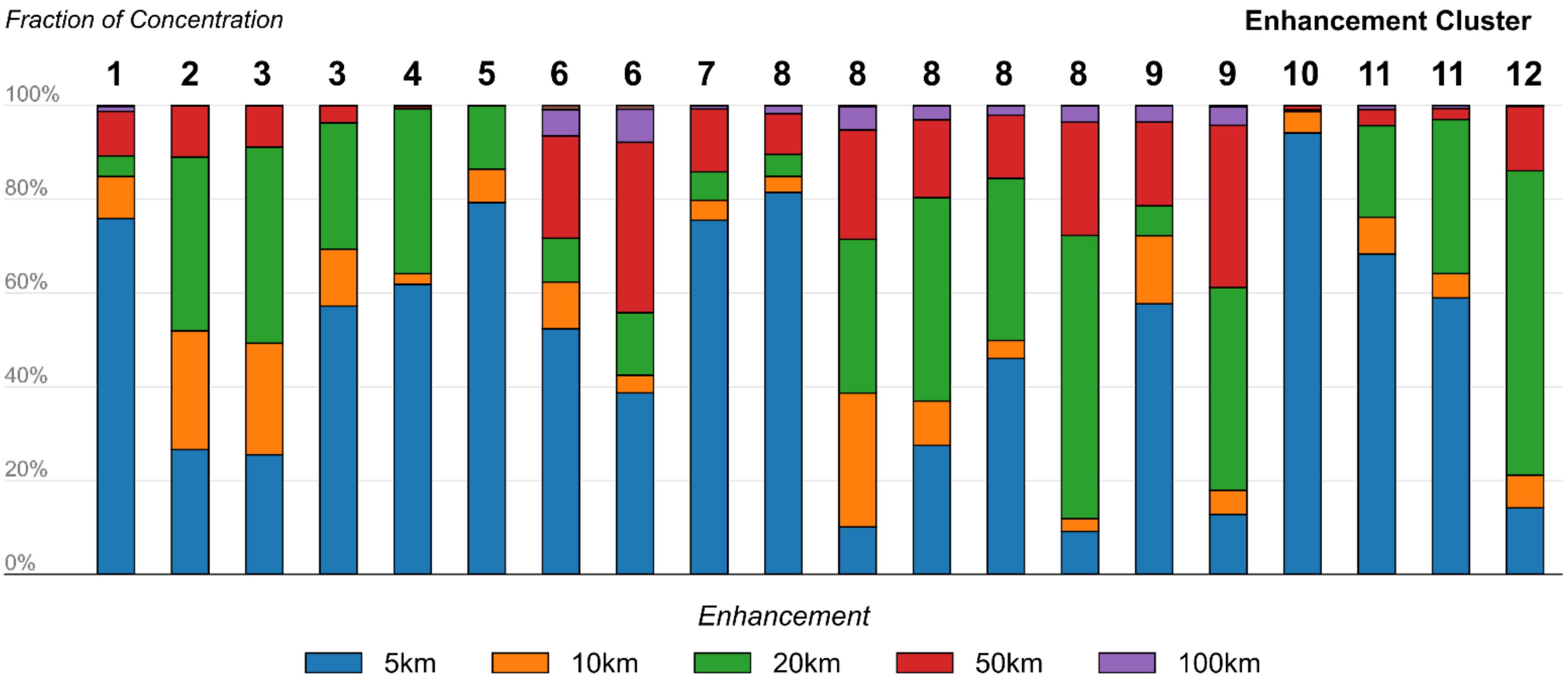



Time Series: Ethane Concentration
Model vs. Observation
Concentration (ppb)
700
600
500
400
300
200
100
0
Model (Routine Emissions)
Observation
Non-Routine
Non-Routine
Non-Routine
03-09
03-16
03-23
03-30
04-06
04-13
Central Standard Time (UTC-6:00)


Distance - Source Contributions
Top 20 Modeled Enhancements - Night
Fraction of Concentration
Enhancement Cluster
1 1 2 2 2 2 2 3 3 3 4 5 5 6 6 6 6 6 7 8
100%
80%
60%
40%
20%
0%
Enhancement
5km
10km
20km
50km
100km

Distance - Source Contributions

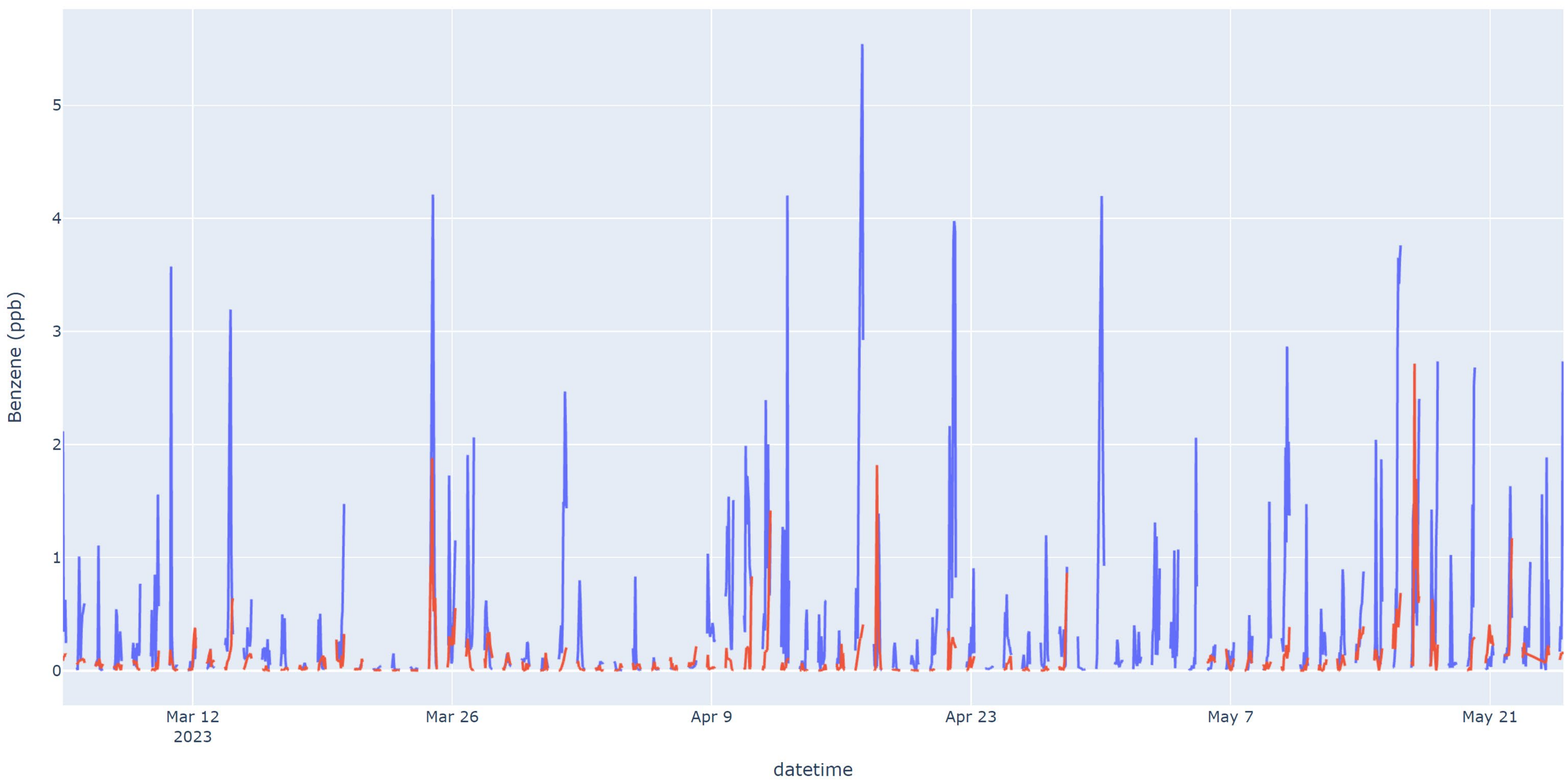
Top 20 Modeled Enhancements - Day



Enhancement clusters are continuous time periods (e.g., cluster 3 is a two hour period with both hours among the top 20 enhancements during the period)

Comparisons of modeling and observations for benzene

Blue: modeled; Red: observed



- Highest modeled and predicted concentrations at night
- Daytime concentrations not shown because of uncertainty in vehicular sources, however, both modeled and predicted concentrations are low
- Over-predictions may be due to over-estimate of benzene content in produced gas in dry gas regions
- Sensitivity analyses to be performed

Key findings

- Elevated concentrations at night dominate exposures
- Mean concentrations at night can be caused by routine emission sources up to 50 km or more from the receptor
- Peak modeled concentrations at night, attributed to routine emissions, are primarily due to sources within 20 km of the receptor
- Large, non-routine emission events are observed, but do not account for a large fraction of the highest concentrations observed at the modeled location in the Eagle Ford production region
- Emissions modeling coupled with dispersion models can be a powerful tool for characterizing exposures

Focus in today's presentation

1. Estimating emissions from UOGD
2. Coupling emissions with dispersion models
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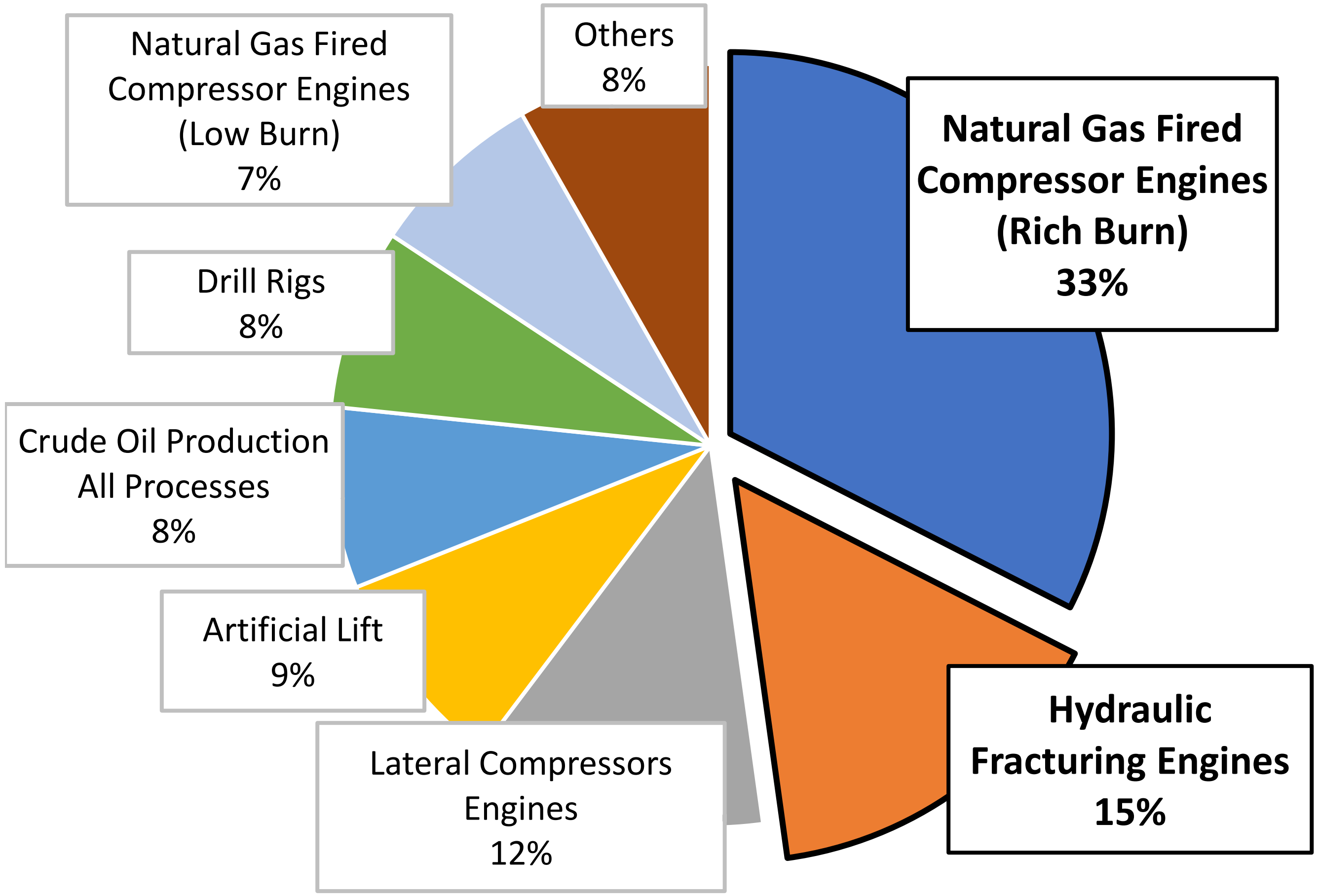
4. Applying the modeling framework to production regions

Emission inventories report NOx emissions from UOGD annually, but they have significant spatial and temporal variability



Distributed broadly across all wells

Operation is near continuous

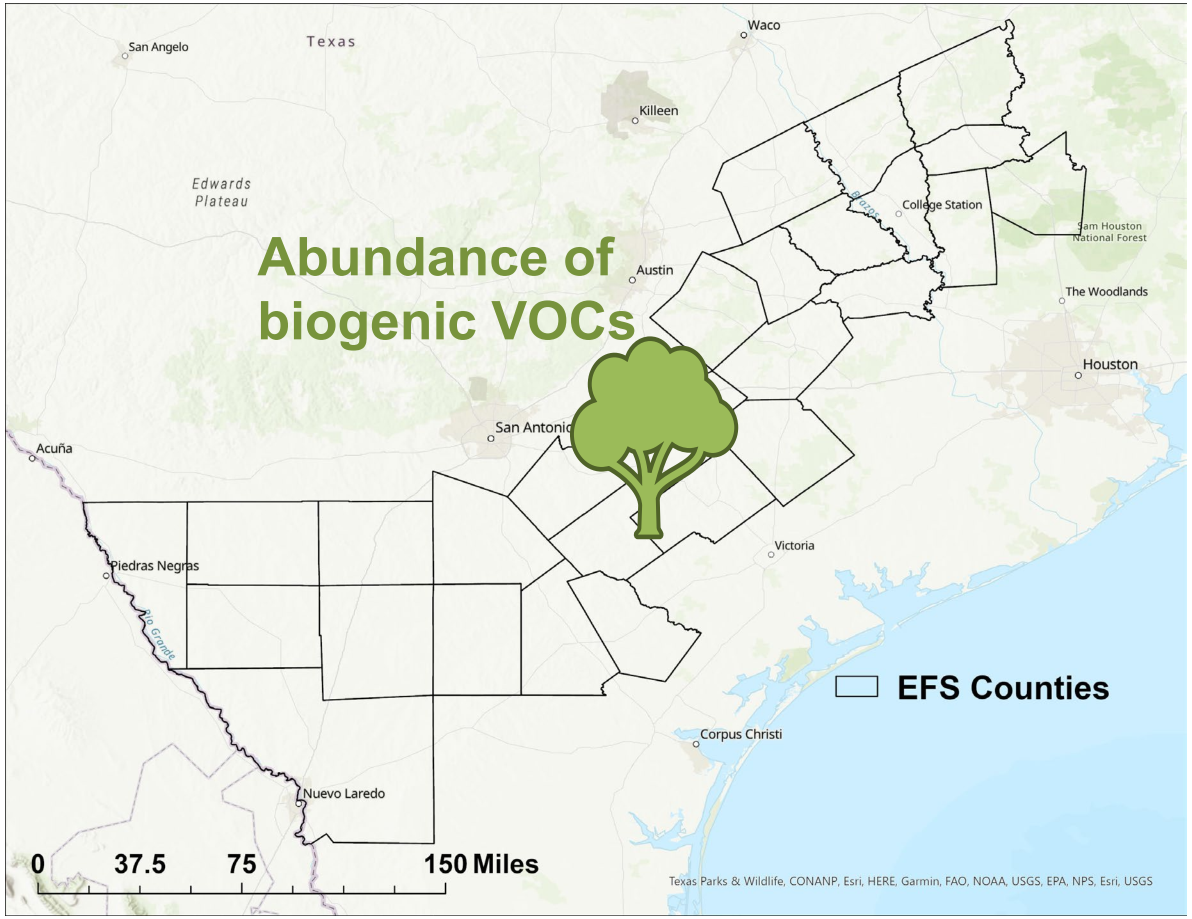
Only at fractured wells (~5% of total)

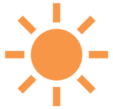
Operational only for 7-10 days

Sources of NOx emissions in the Eagle Ford Shale

NEI, 2020

NOx Emissions from UOGD in the Eagle Ford Shale have the potential to drive significant ozone formation



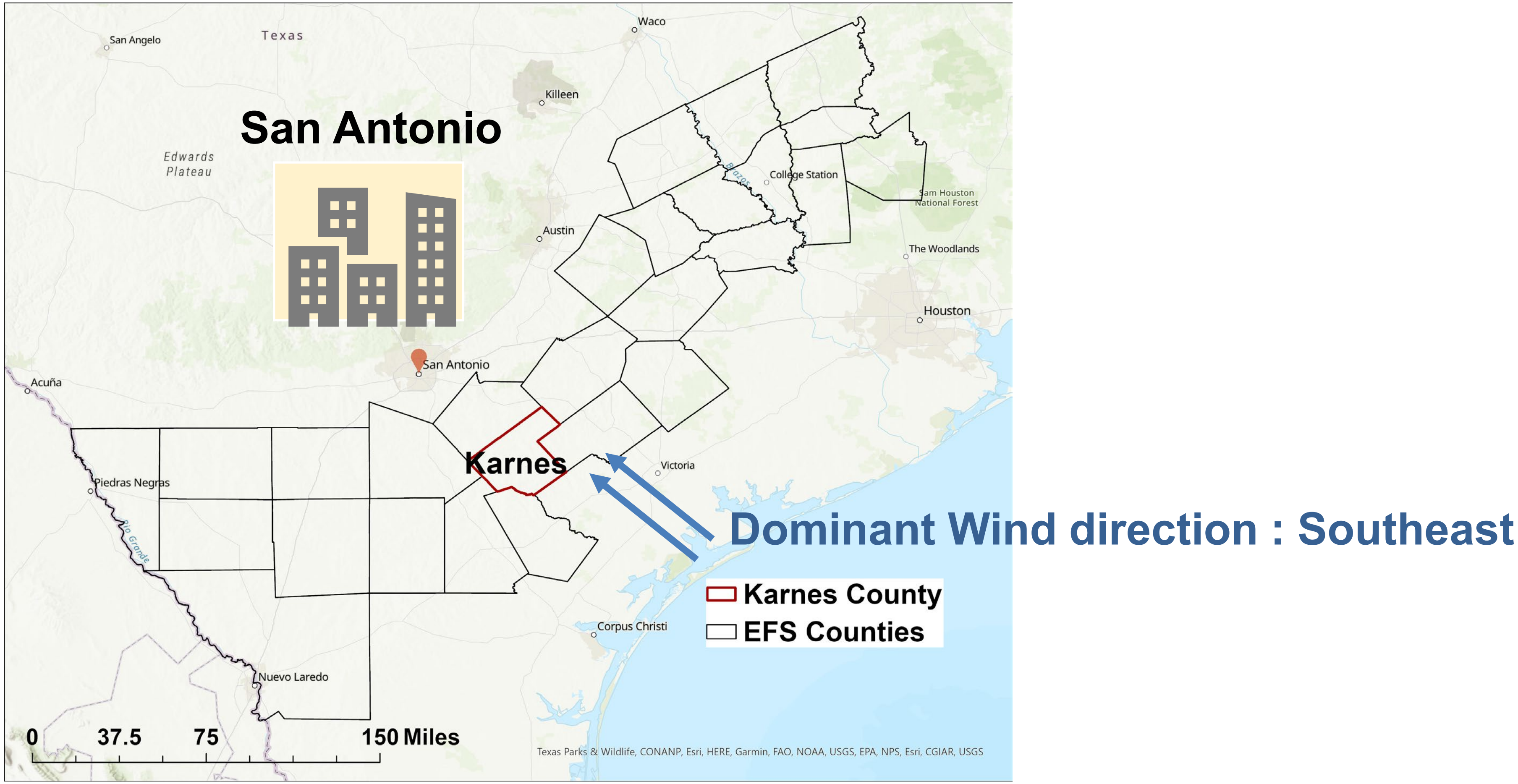


$VOCs + NOx \rightarrow O_3$

The extent of ozone formation in Eagle Ford Shale depends on the spatial and temporal distributions of the NOx emissions.

Wiedinmyer et al., 2001 and Yu et al., 2017

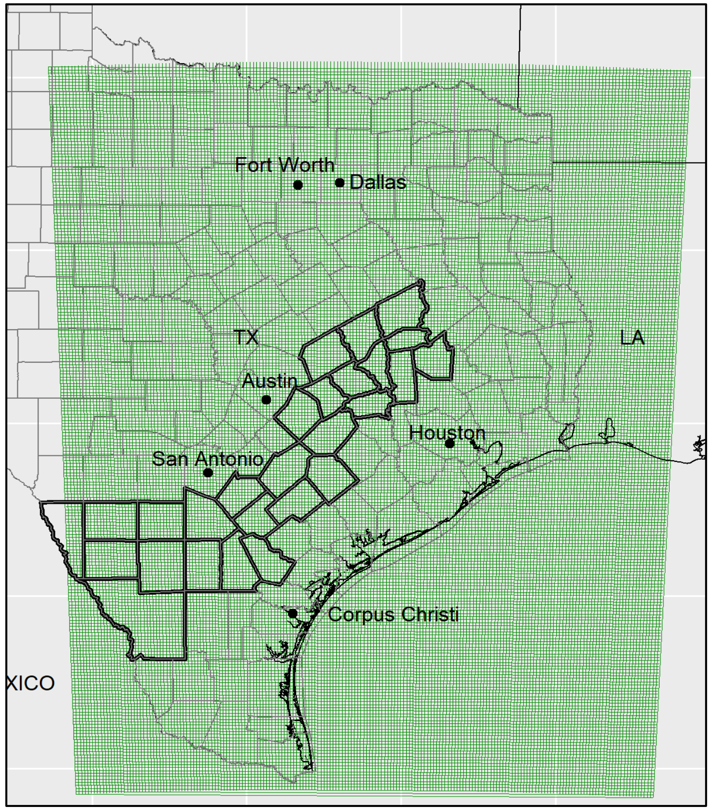
What is impact of NOx emissions from hydraulic fracturing in Karnes County on regional ozone formation in San Antonio?



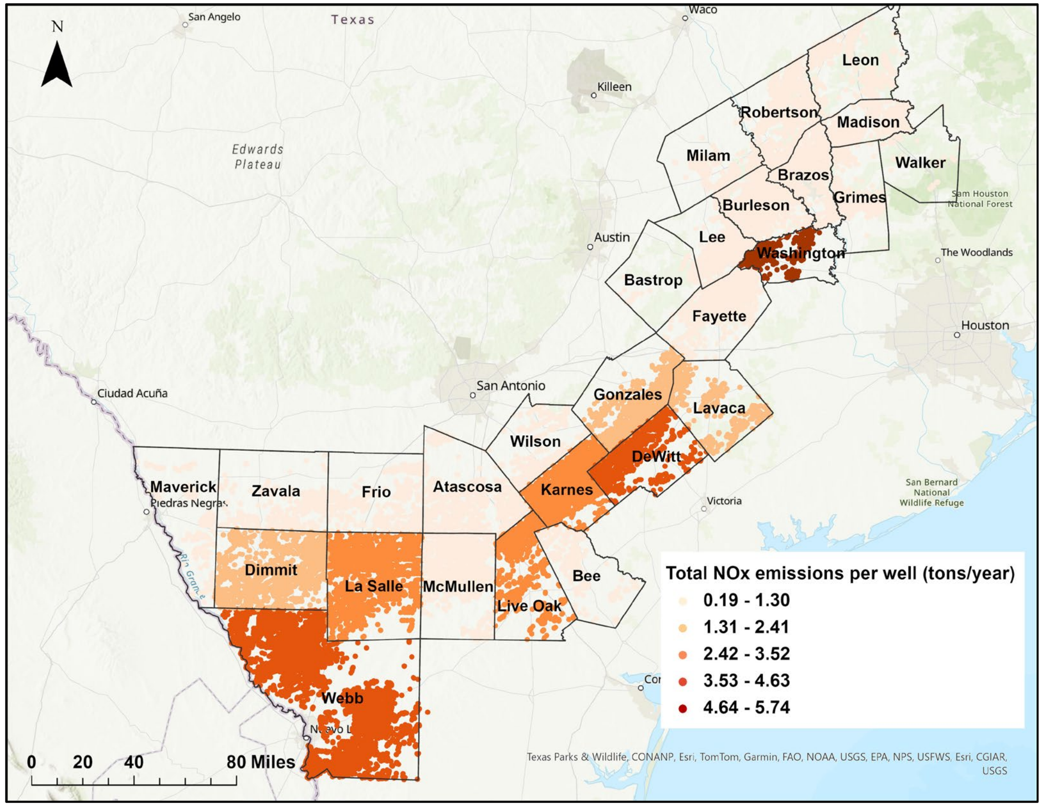
Karnes County accounts for 25% of the NOx emissions from hydraulic fracturing in Eagle Ford Shale

TCEQ (2021); NEI (2020); Pacsi et al. (2015)

Case 1 : Allocated NOx emissions evenly to all active oil and gas wells within each of the Eagle Ford Shale counties



Removed NOx emissions from Texas Commission on Environmental Quality (TCEQ) 2019 Base Case Inventory



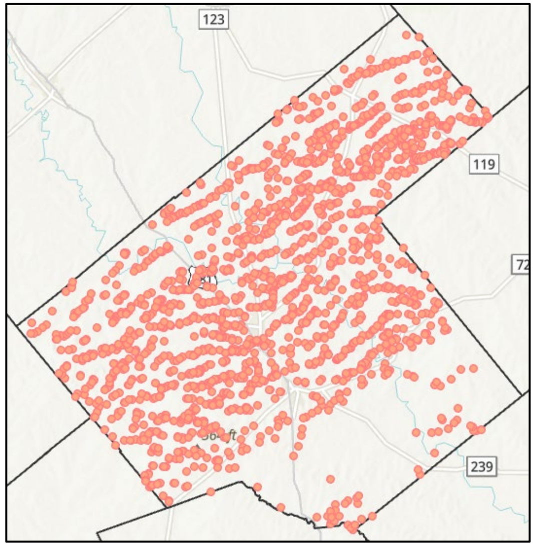
Case 1: All wells in the Eagle Ford Shale counties emit NOx continuously throughout the year

TCEQ (2023); TRRC (2023)

Cases 2-4 : Allocating NOx emissions from hydraulic fracturing only to fractured wells at various temporal scales in Karnes County

1960 tons/year of Hydraulic Fracturing NOx emissions (2019)

Case 1 : Annual even allocation

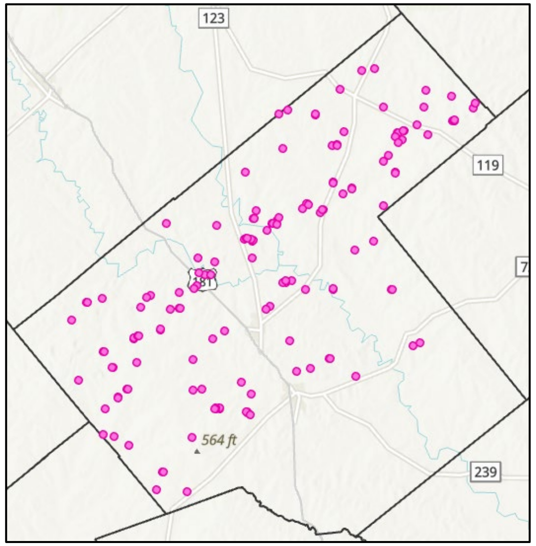


4185 oil and gas wells in Karnes
365 days

0.001 tons/day per well

436 wells were fractured in Karnes in 2019

Cases 2-4 : Detailed allocation



436 fractured wells
Case 3 : 7 days prior completion

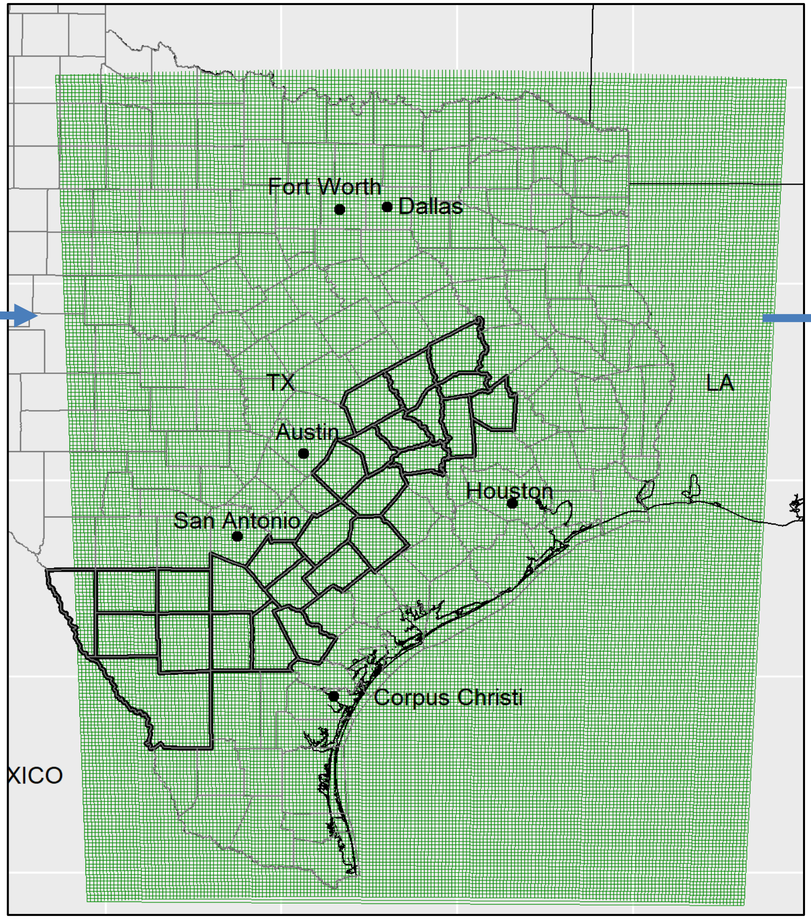
0.6 tons/day per fractured well

Emission Duration :
Case 2 : 14 days
Case 3 : 7 days
Case 4 : 2 days

Different allocation methods of NOx emissions from hydraulic fracturing, result in NOx emission rates varying by **two to three orders of magnitude**.

Metrics for evalauting ozone concentrations

Emission Scenarios (Case 1 - 4)



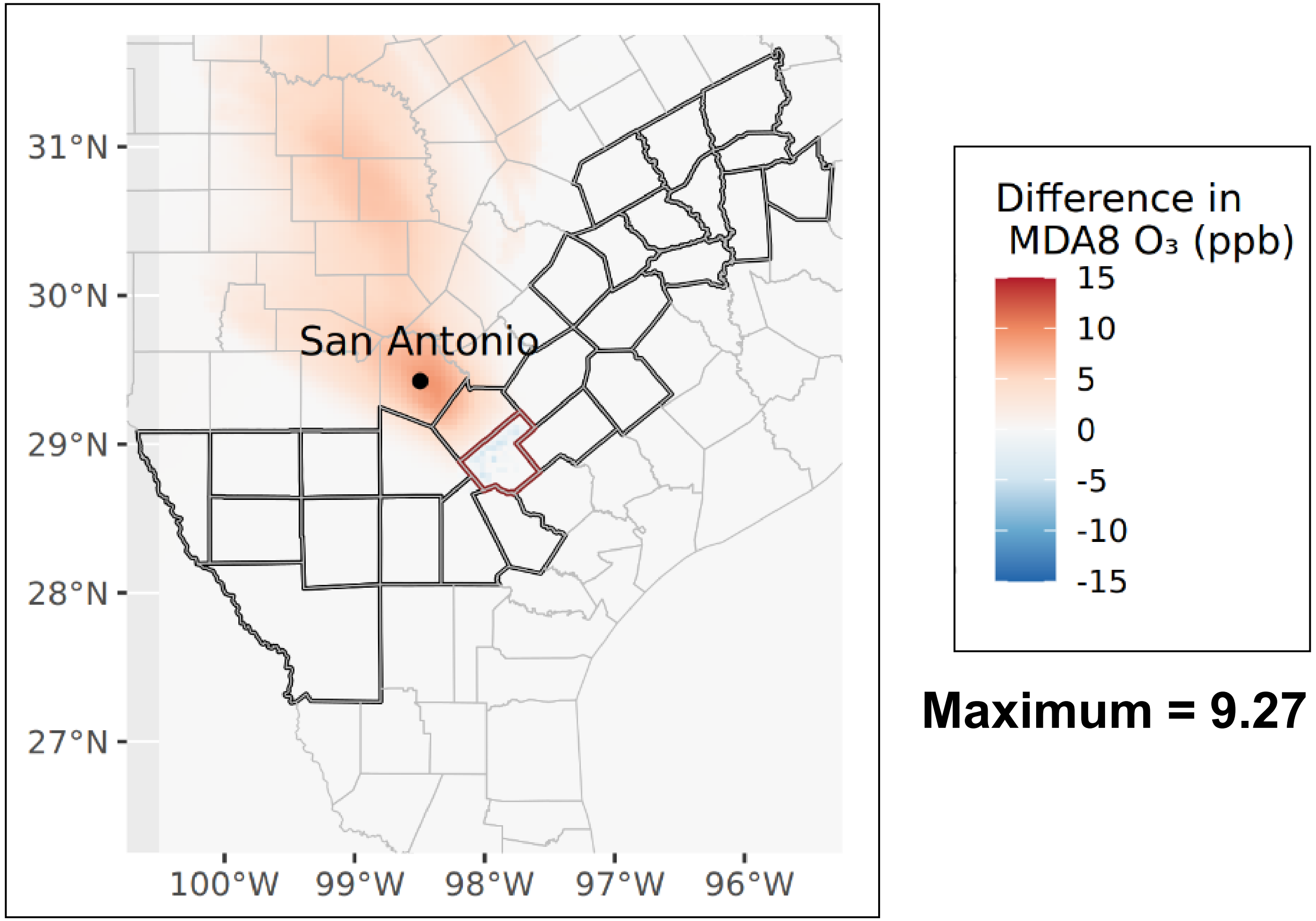
Comprehensive Air Quality Model with Extensions (CAMx) for April – Oct 2019

Hourly ozone concentrations at all grid cells

Daily Maximum of 8-h average (MDA8) O_3 concentrations (ppb) at all grid cells

Differences in MDA8 O_3 all between Case 3 (detailed allocation) and Case 1 (annual even allocation)

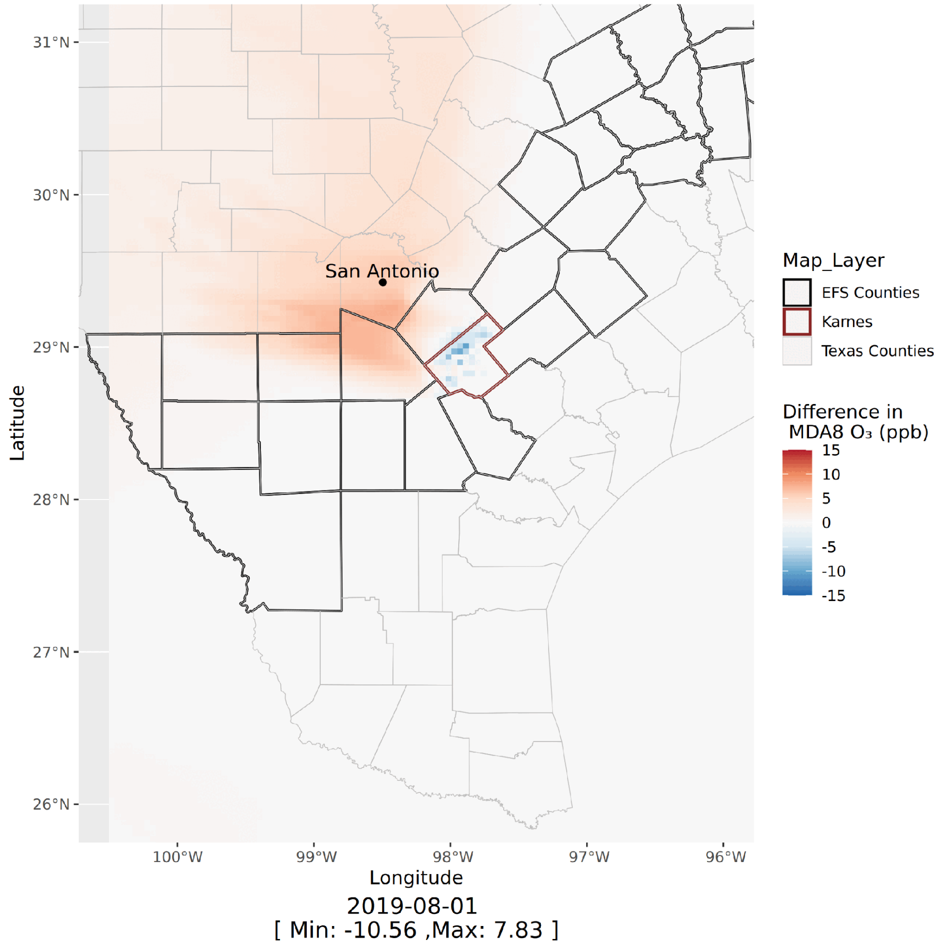
Detailed allocation of NOx emissions from hydraulic fracturing results in increased regional ozone formation



Maximum = 9.27 ppb

Differences in MDA8 O_3 concentrations on August 27, 2019
Detailed allocation (Case 3) - Annual even distribution (Case 1)

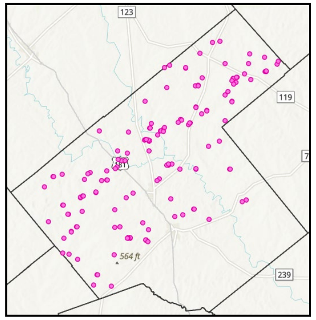
Ozone concentrations were consistently 8 to 10 ppb higher for detailed allocation during August

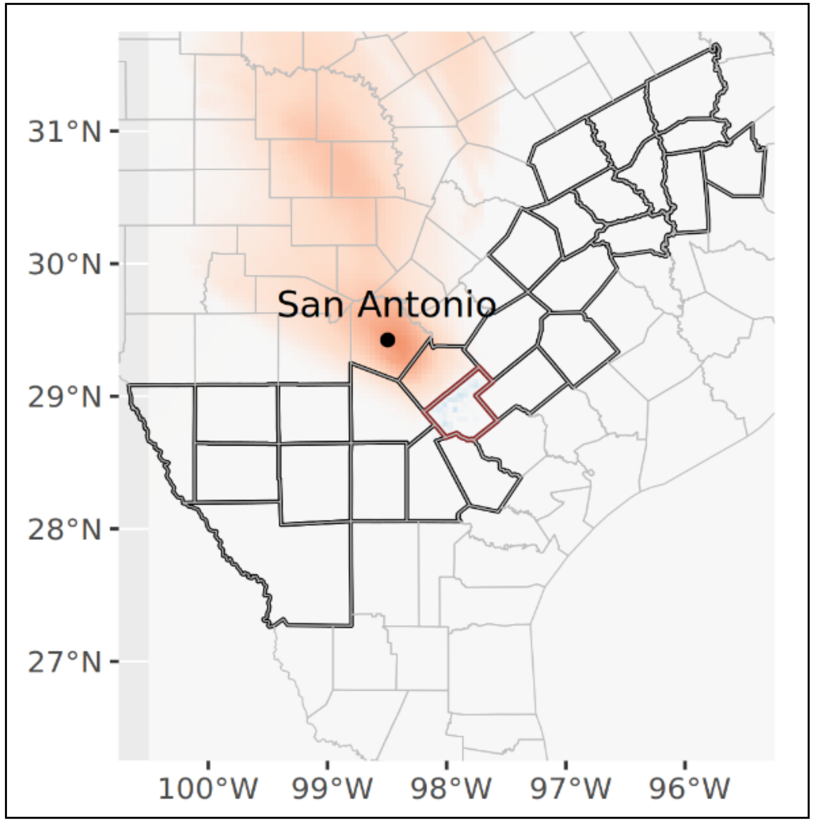


National Ambient Air Quality Standards NAAQS for Ozone :
70 ppb (3-year average of the annual fourth-highest MDA8 O_3)

Key Findings

- UOGD activities like hydraulic fracturing are highly localized and episodic : only occur at **selected well-sites** and last only for **1-2 weeks prior** to production.
- Different allocation methods of NOx emissions from hydraulic fracturing result in NOx emission rates varying by **two to three orders of magnitude.**
- **Fine scale spatial and temporal allocation** of NOx emissions from hydraulic fracturing results in **increased predicted ozone formation** in the Eagle Ford Shale, a NOx-limited oil and gas production region.
- These results have air quality and human health implications for San Antonio, the seventh most populous city in the US.
- Similar results can be expected for drilling activity.



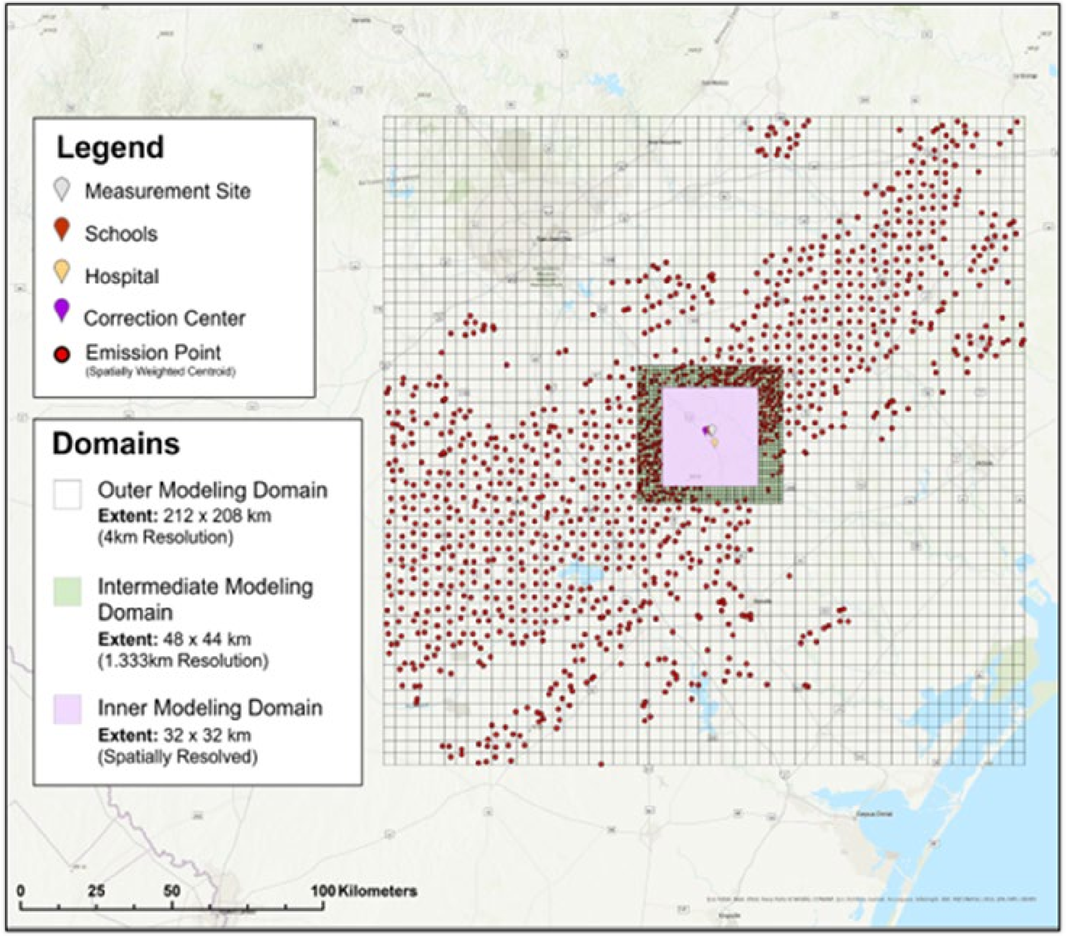


Focus in today's presentation

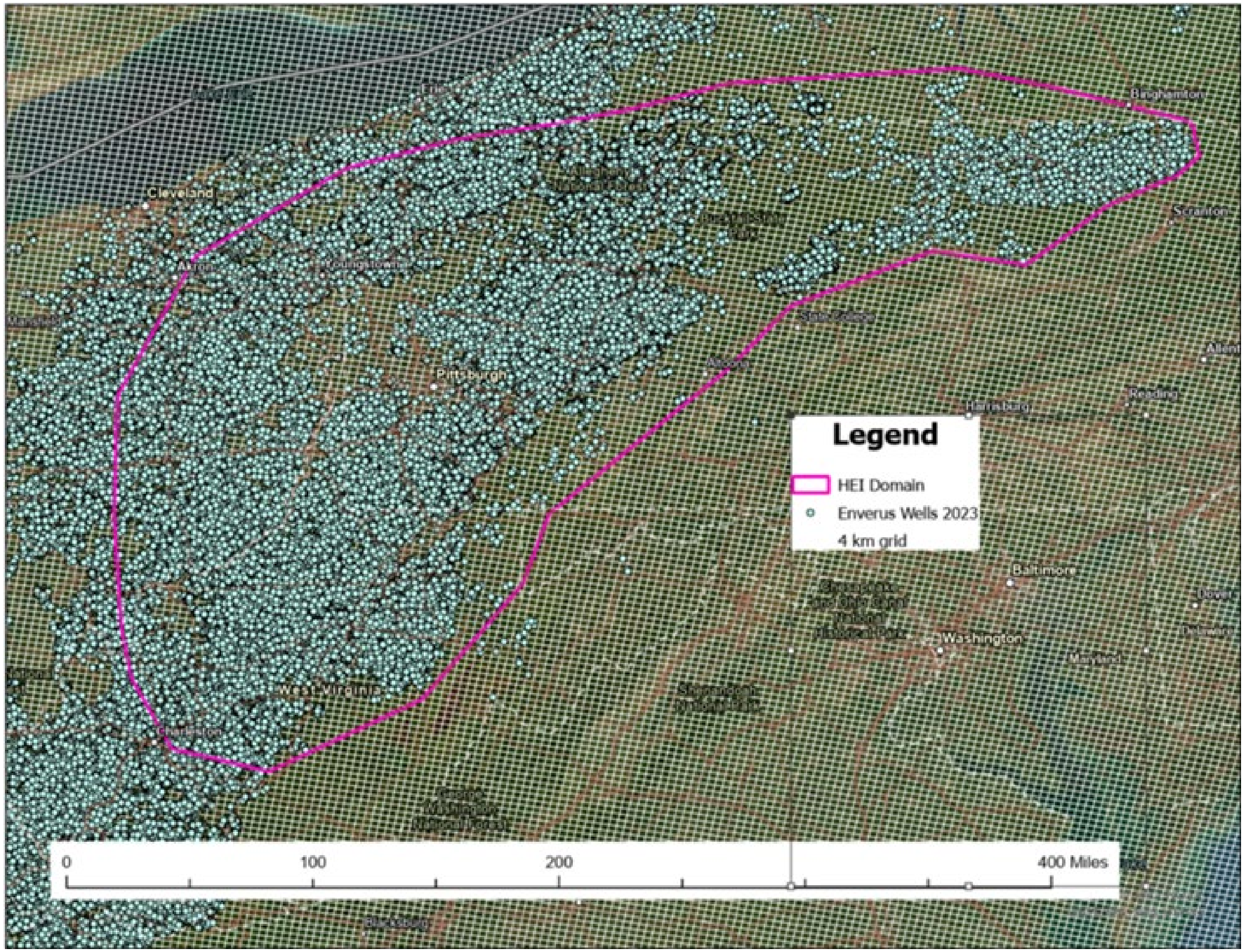
1. Estimating emissions from UOGD
2. Coupling emissions with dispersion models
3. Coupling emissions with chemical transport models
4. Applying the modeling framework to production regions

Develop gridded inventories at fine spatial and temporal resolution; characterize spatial and temporal variability

Eagle Ford

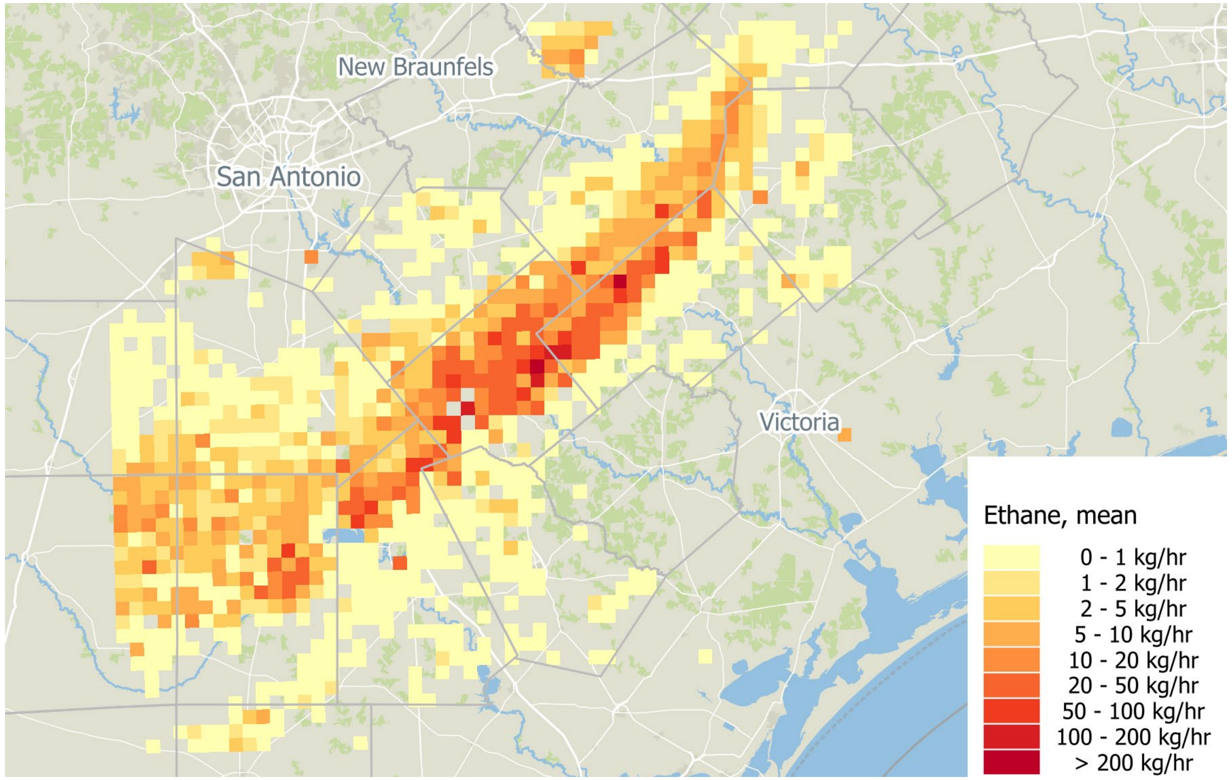


Marcellus

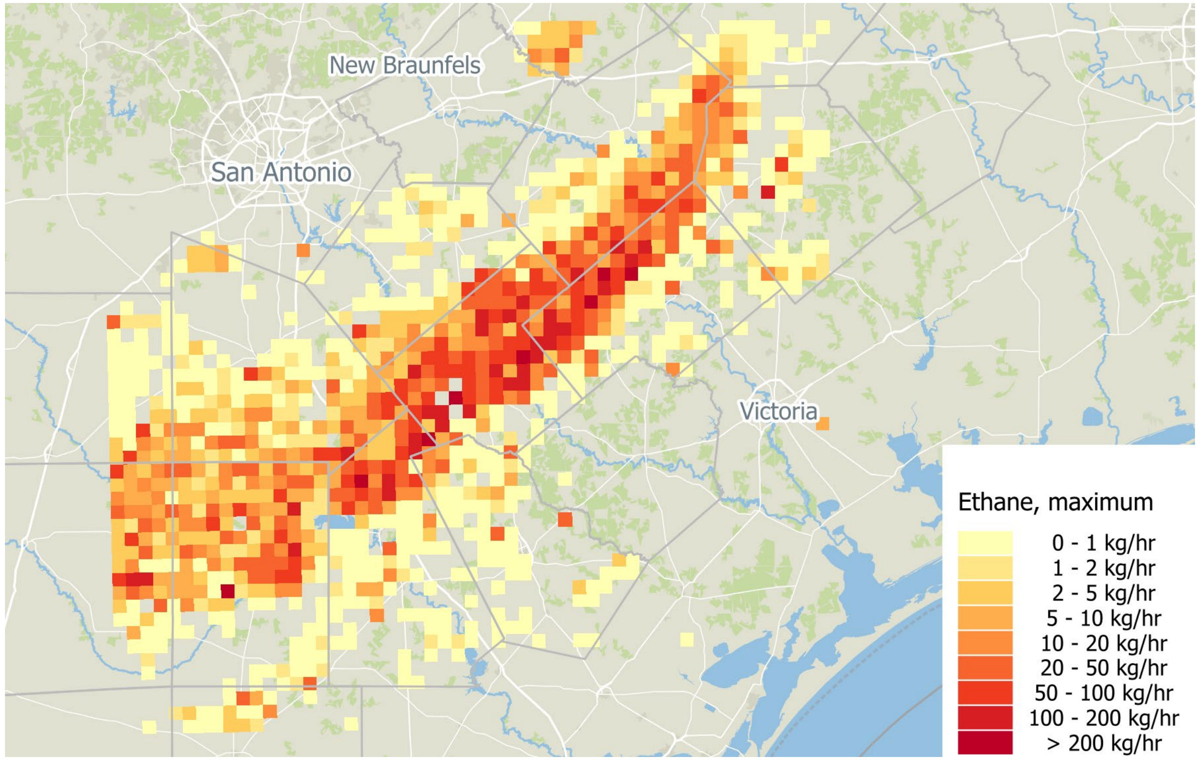


Eagle Ford inventory mappings: ethane

Average emission rates

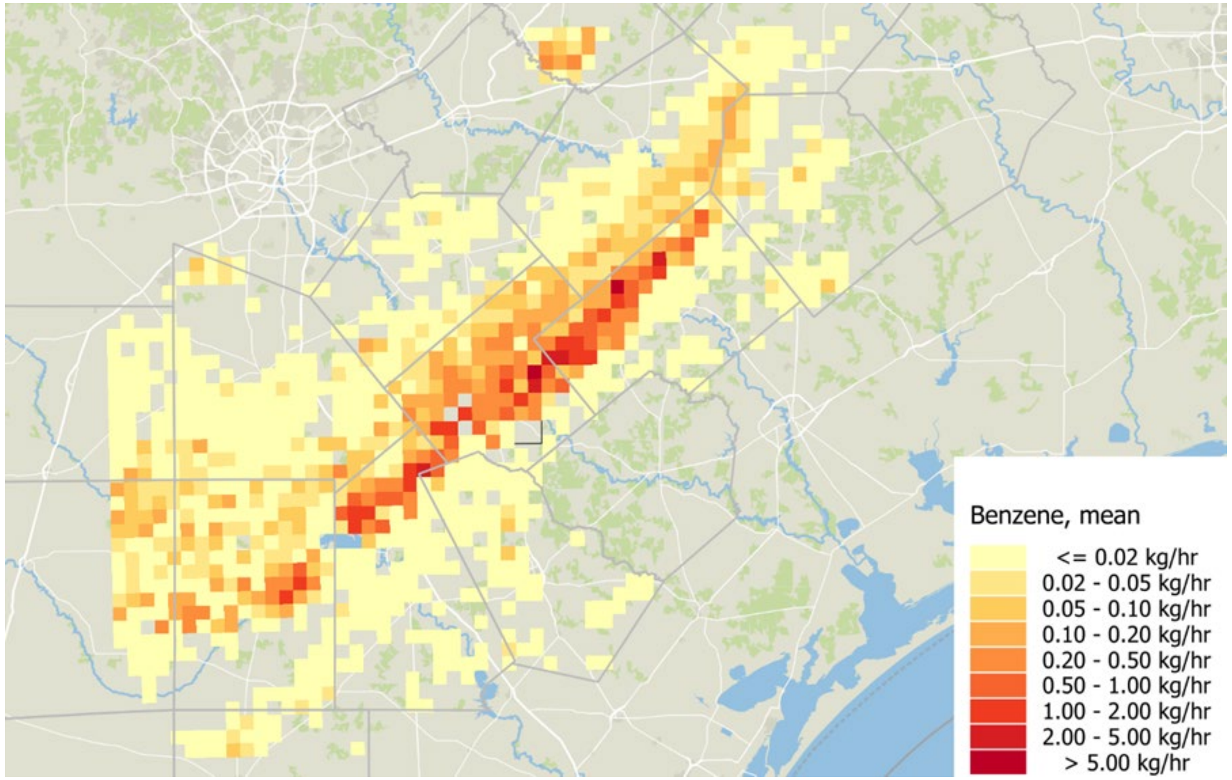


Maximum emission rates

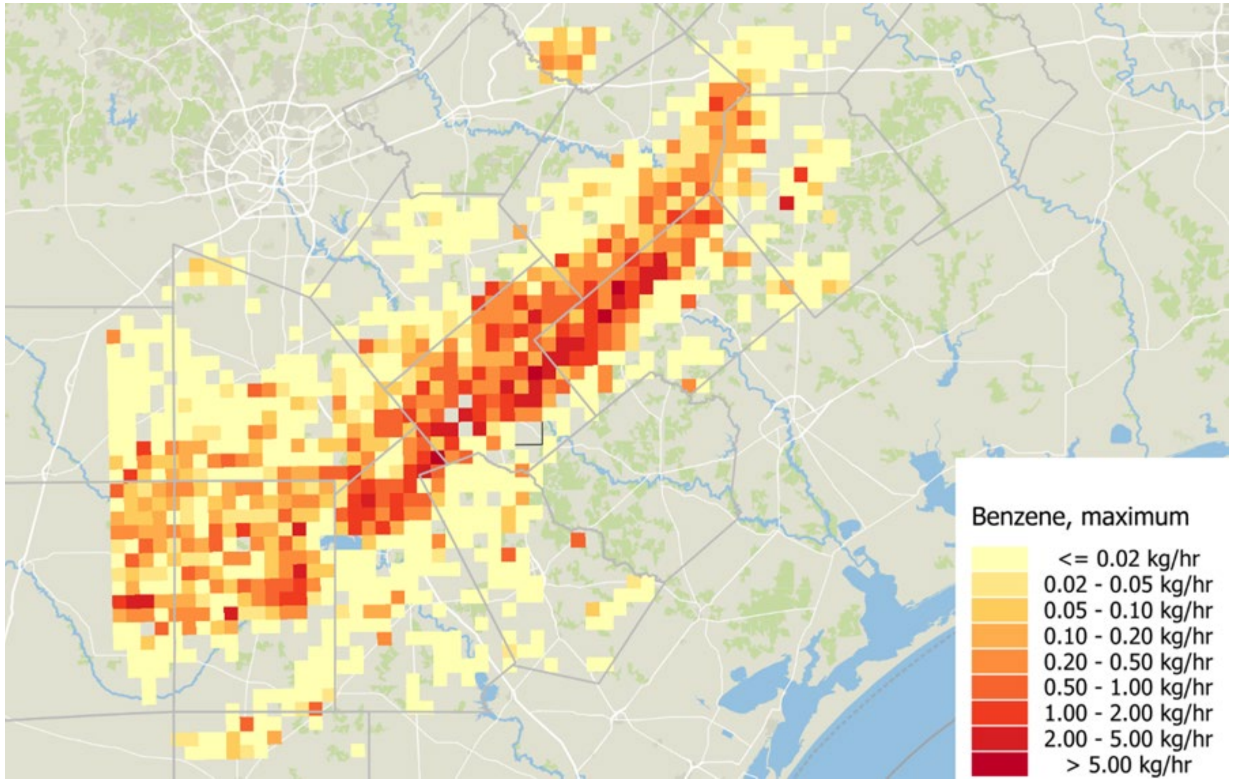


Eagle Ford inventory mappings: benzene

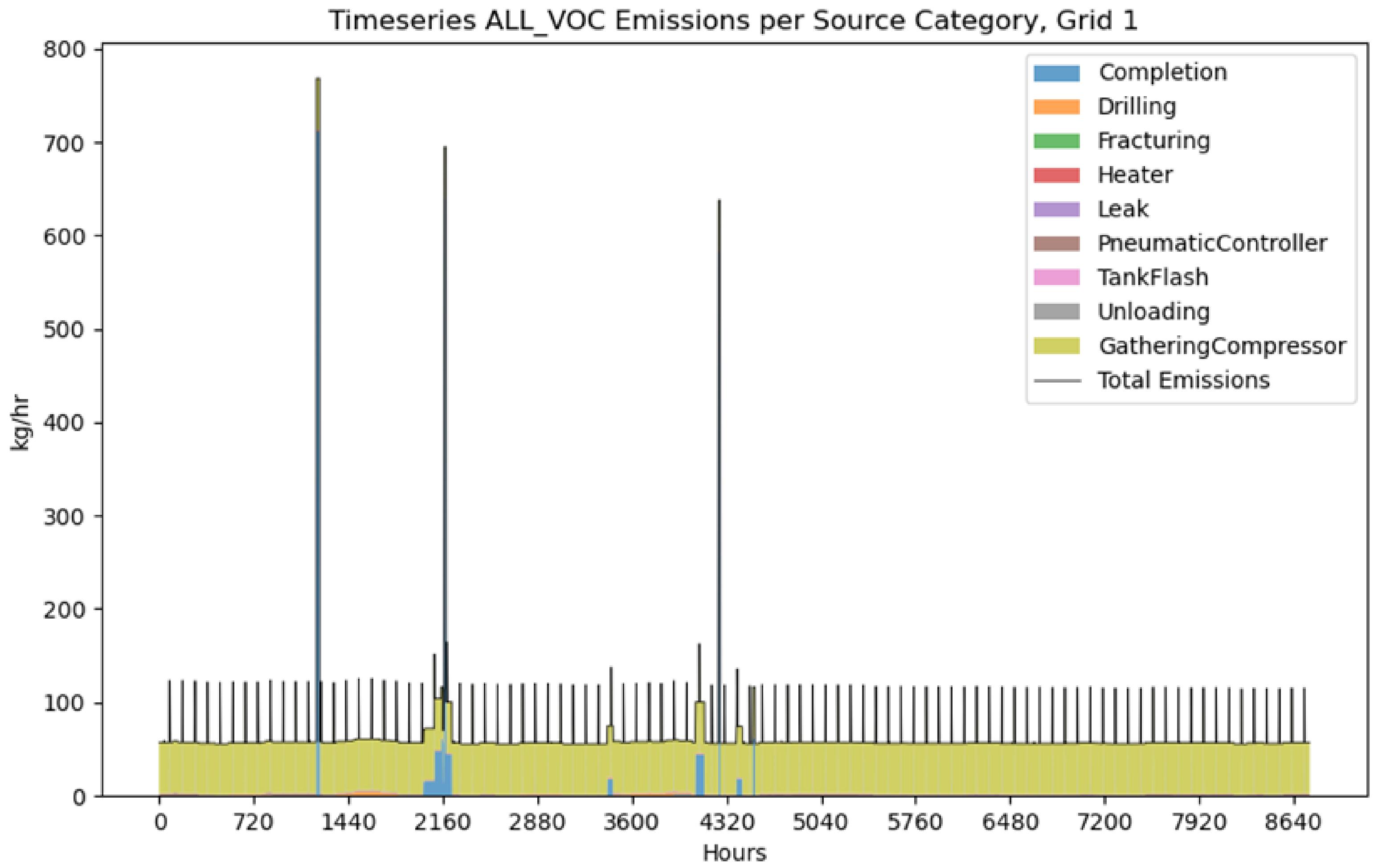
Average emission rates



Maximum emission rates



Marcellus inventory grid cells: Hourly time series of individual grid cell VOC emissions



Focus in today's presentation

1. Estimating emissions from UOGD
2. Coupling emissions with dispersion models
3. Coupling emissions with chemical transport models
4. Applying the modeling framework to production regions