



Cornell University

Near-Road Air Quality Monitoring and Modeling: Towards a Mechanistic Understanding

K. Max Zhang

Energy and the Environment Research Laboratory
Sibley School of Mechanical and Aerospace Engineering

Outline

- An integrated monitoring and modeling approach for studying near-road air quality
- Development of CFD-VIT-RIT modeling system, an advanced project-level analysis tool
- Applications of CFD-VIT-RIT in project-level analysis
 - Spatial gradients of air pollutants near elevated highways
 - Chemical evolution of NO_2 near roadways
- Discussions

Near-road air pollution: Health effects and human exposure

New York: A large number of New York residents live within 150m and 300m of major roads in urban, suburban, and even rural counties.

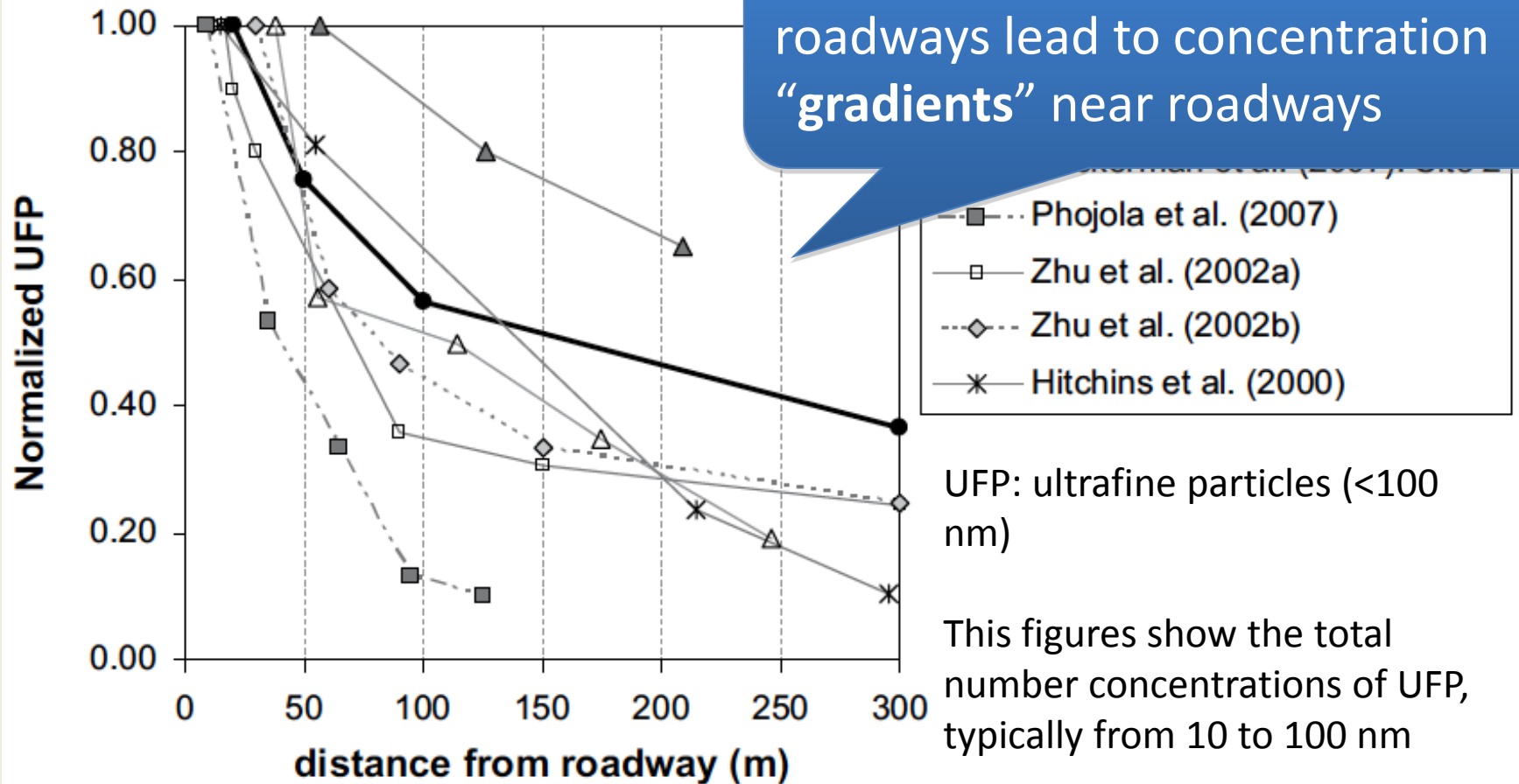
NYS counties	entire county (number)	Population (%)		
		residential distance to major road		
		<150 m	150-300 m	<300 m
Urban				
Bronx	1,074,102	66%	25%	91%
New York	1,571,892	95%	5%	100%
Queens	2,120,944	28%	60%	88%
Suburban				
Nassau	1,284,267	43%	30%	74%
Westchester	857,975	43%	29%	72%
Rural				
Cattaraugus	85,702	22%	19%	41%
Greene	47,851	17%	12%	28%
Lewis	26,926	13%	11%	24%

Rationales for an integrated monitoring and modeling approach

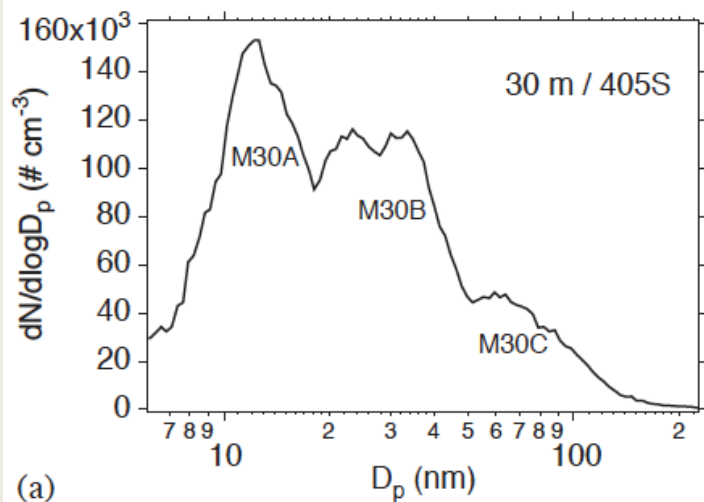
- The atmospheric processes at project-level are complex, governing the transport and transformation of multiple air pollutants, which in turns determine their concentrations near roadways.
- Road design features such as alternative highway configurations and presence of roadside structures further influence the pollutant transport and transformation.
- The current project-analysis tools based on Gaussian plume models are not capable of handling complex roadway environments. Advanced modeling tools are needed.
- Advanced modeling tools can be used to interpret monitoring results and predict future near-road air quality

Characterizing near-road air pollution

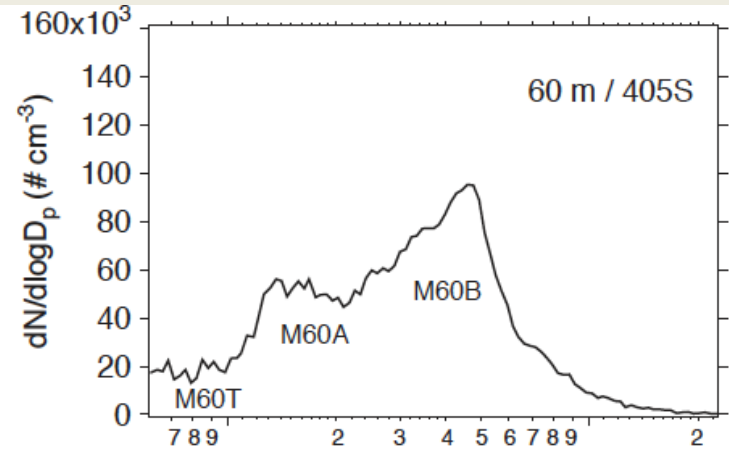
Elevated air pollution levels near roadways lead to concentration “gradients” near roadways



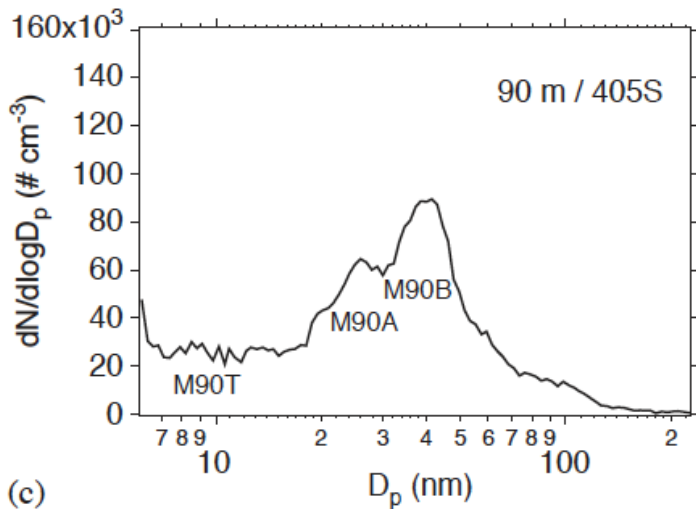
Characterizing near-road air pollution



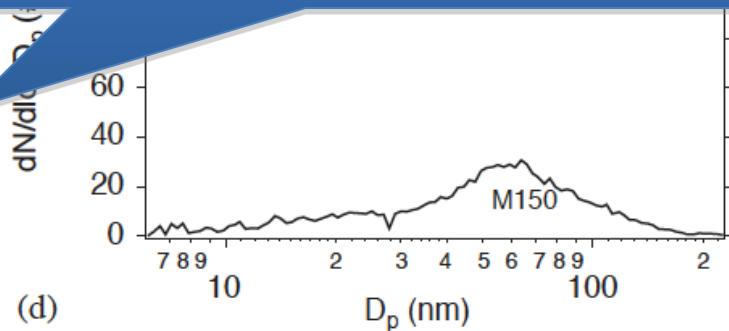
(a)



Reactive and volatile species undergo chemical and/or physical transformation near roadways

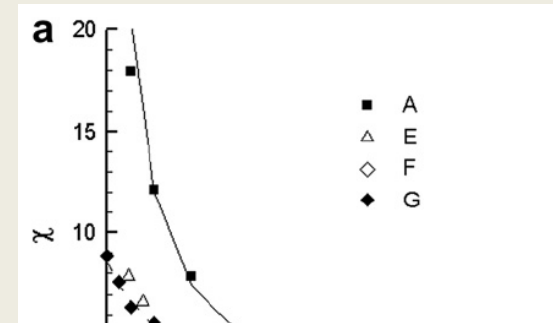
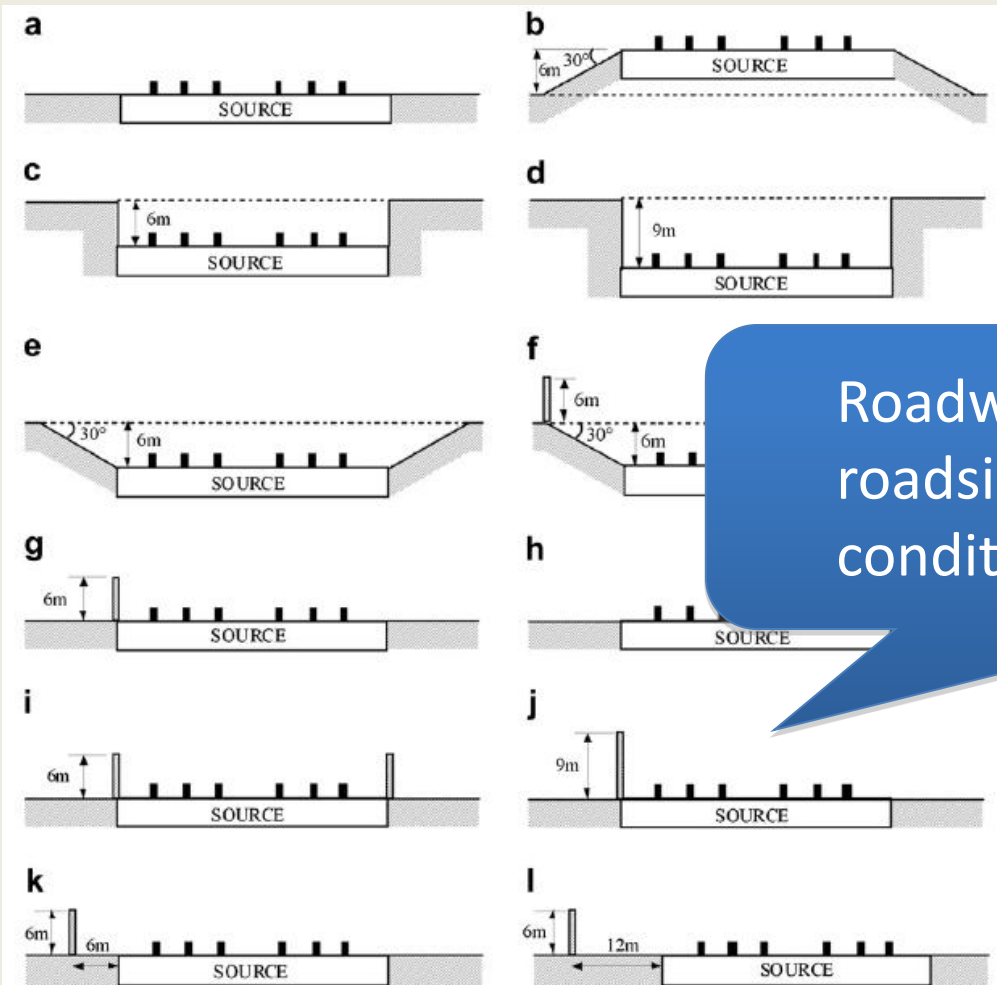


(c)

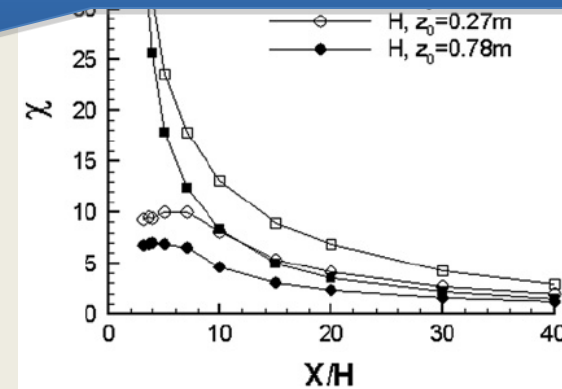


(d)

Noise barriers and road configurations



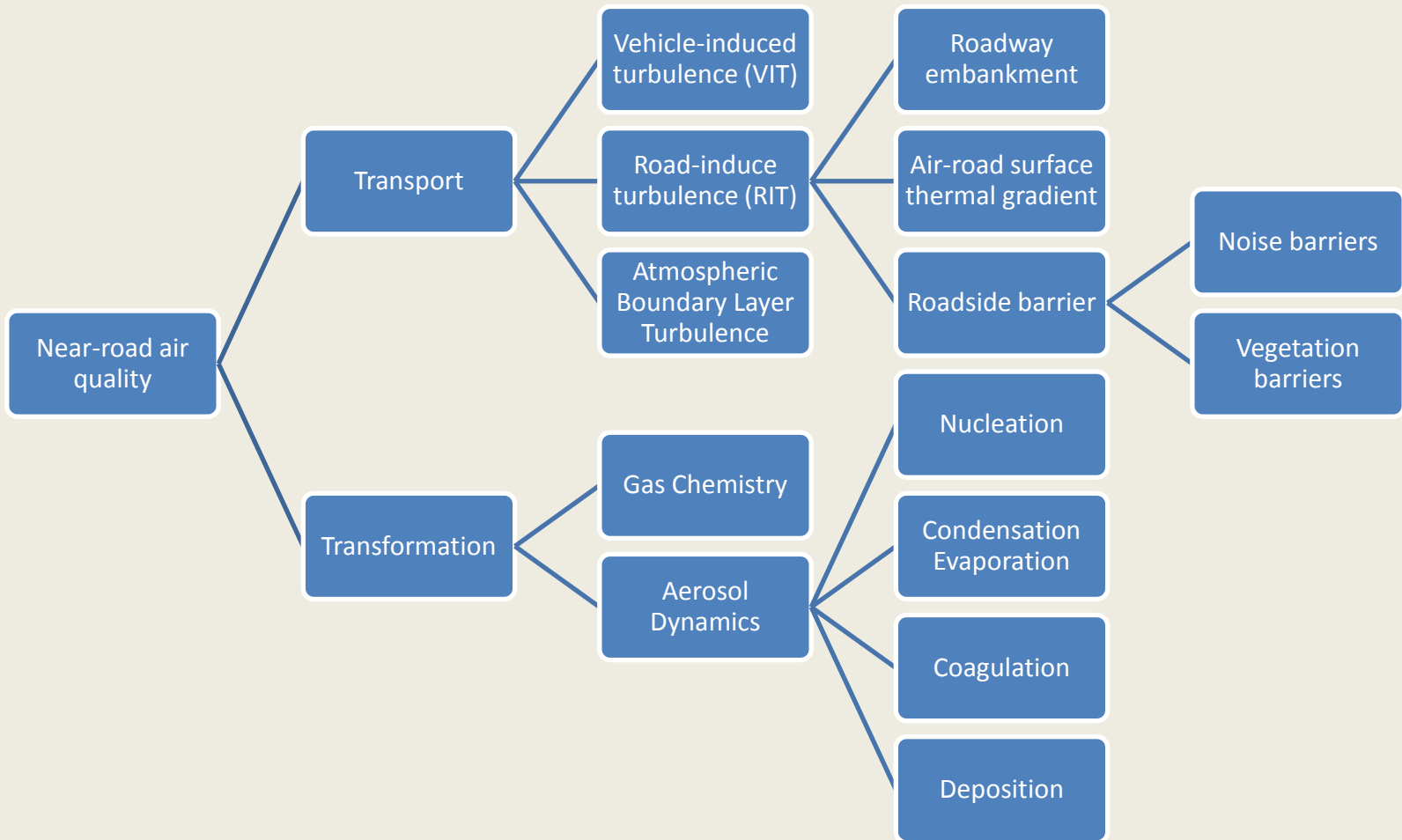
Roadway configuration, presence of roadside barriers and meteorological conditions affect the gradients



Rationales for an integrated monitoring and modeling approach

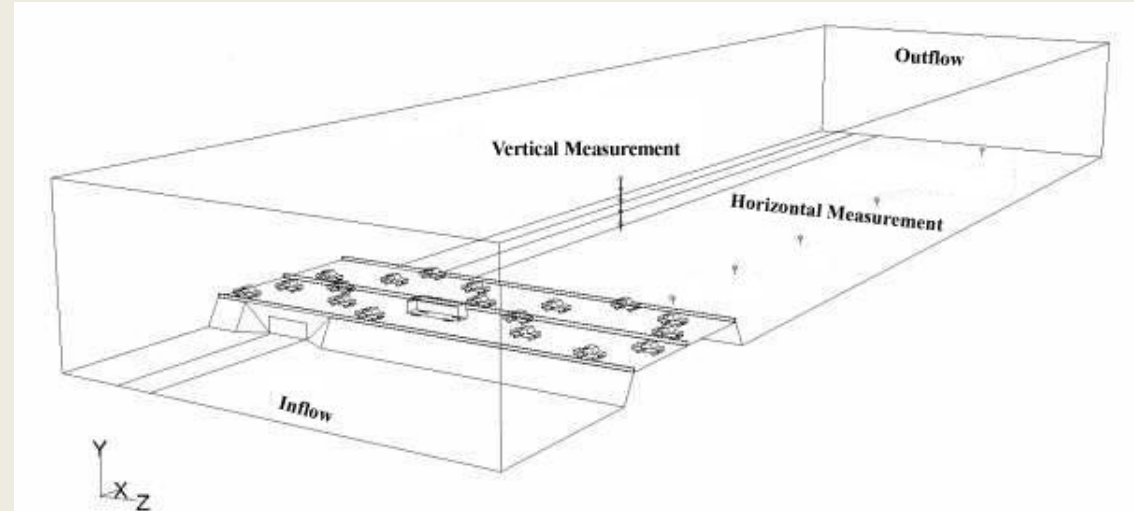
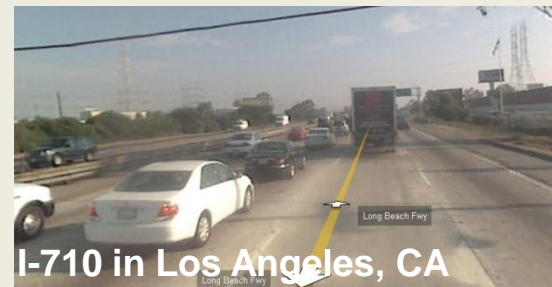
- The atmospheric processes at project-level are complex, governing the transport and transformation of multiple air pollutants, which in turns affect their health effects near roadway
- Road configuration and roadway geometry influence near-road air quality. The nature of near-road air quality is 3-D turbulent reacting flows, coupling of transport and transformation
- The current project-analysis tools based on Gaussian plume models are not capable of handling complex roadway environments. Advanced modeling tools are needed.
- Advanced modeling tools can be used to interpret monitoring results and predict future near-road air quality

CFD-VIT-RIT, a micro-environmental air quality model for project-level analysis



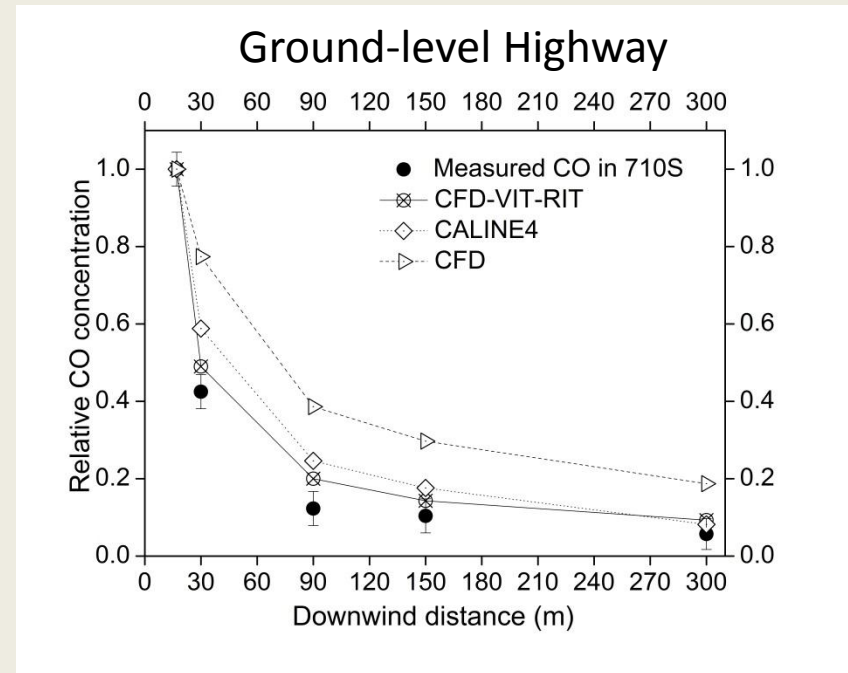
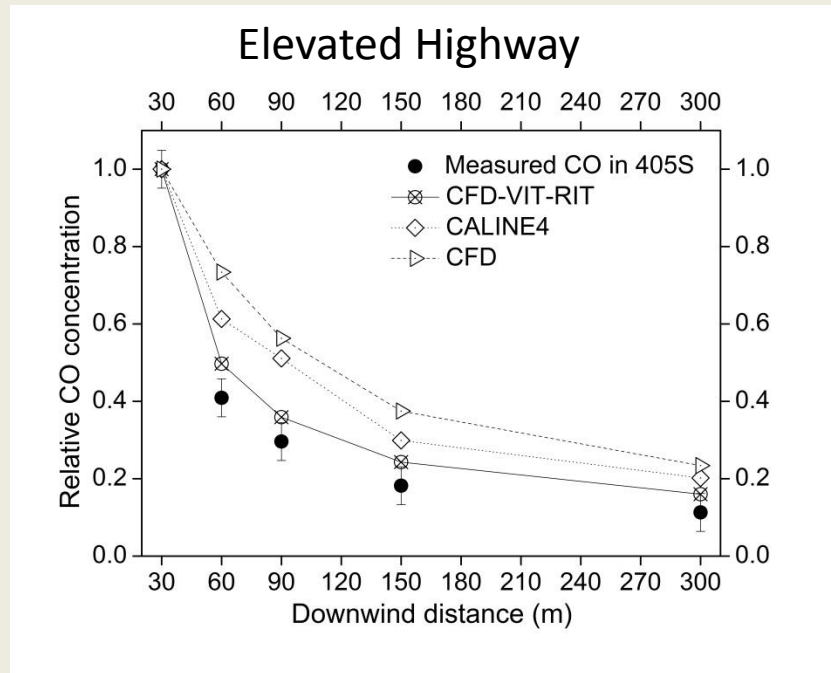


CFD-VIT-RIT: Roadway configurations



- We employed a Reynolds-averaged Navier–Stokes (RANS) model to simulate the turbulent mixing processes on and near roadways.
- The moving vehicles were modeled as moving walls with surface roughness to capture the vehicle-induced turbulence (VIT).
- We built the highway geometry to represent the realistic shape with elevated surface temperature to capture the road-induced turbulence (RIT).

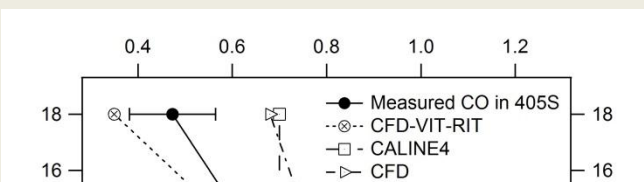
CFD-VIT-RIT: Horizontal gradients



- CALINE4 appears to be adequate in capturing the horizontal gradients of inert species
- For ground-level highway, the predictions from CALINE4 and CFD-VIT-RIT are almost identical.

CFD-VIT-RIT: Veridical gradients

Elevated Highway



Ground-level Highway

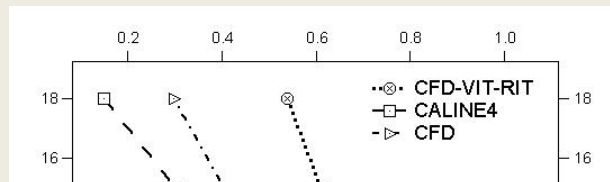


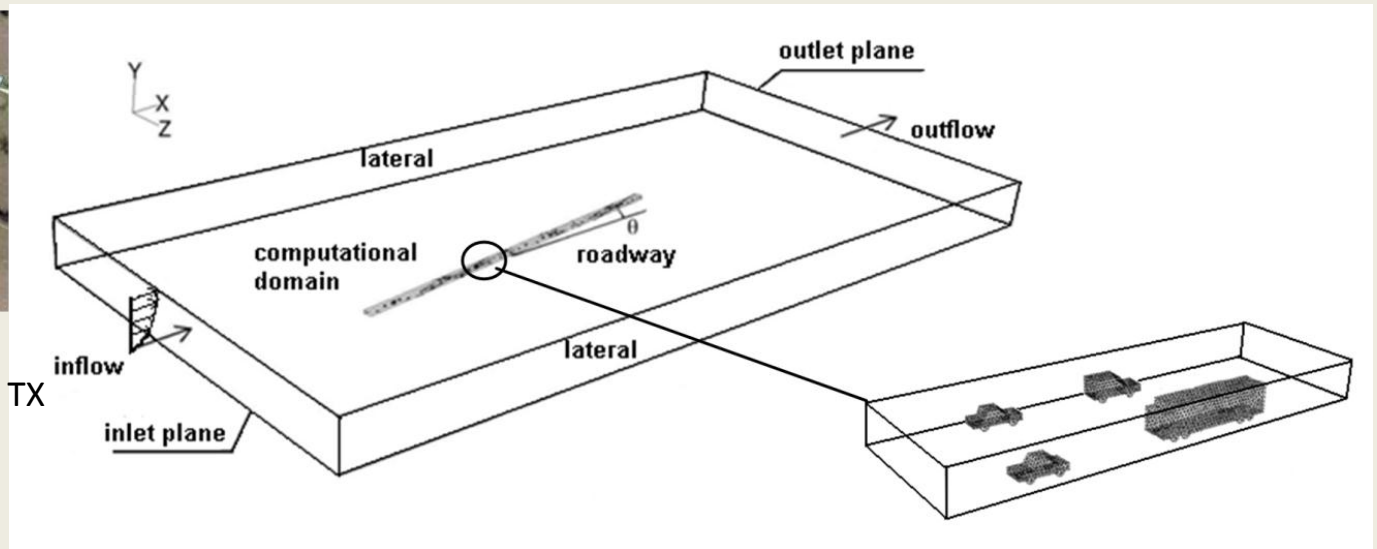
TABLE 1. Summary of TKE in the Test Zone

	I-405				I-710			
	summer	percentage	winter	percentage	summer	percentage	winter	percentage
VIT ^a	0.36	41.4%	0.35	53.9%	0.63	76.8%	0.63	95.5%
RIT - embankment ^a	0.30	34.5%	0.27	41.5%	N/A	N/A	N/A	N/A
RIT - thermal effects ^a	0.17	19.5%	N/A	N/A	0.15	18.3%	N/A	N/A
ABLT ^a	0.04	4.6%	0.03	4.6%	0.04	4.9%	0.03	4.5%
total TKE ^a	0.87	100.0%	0.65	100.0%	0.82	100.0%	0.66	100.0%

^a Unit is $m^2 s^{-2}$.

- Due to its rigorous treatment of turbulence mixing mechanisms, CFD-VIT-RIT is able to capture the vertical gradient of inert species near elevated highways. The prediction from CALINE4 appears to be inadequate.
- A CFD model without detailed treatment of VIT and RIT adds no more benefits than CALINE4 besides high computational cost.

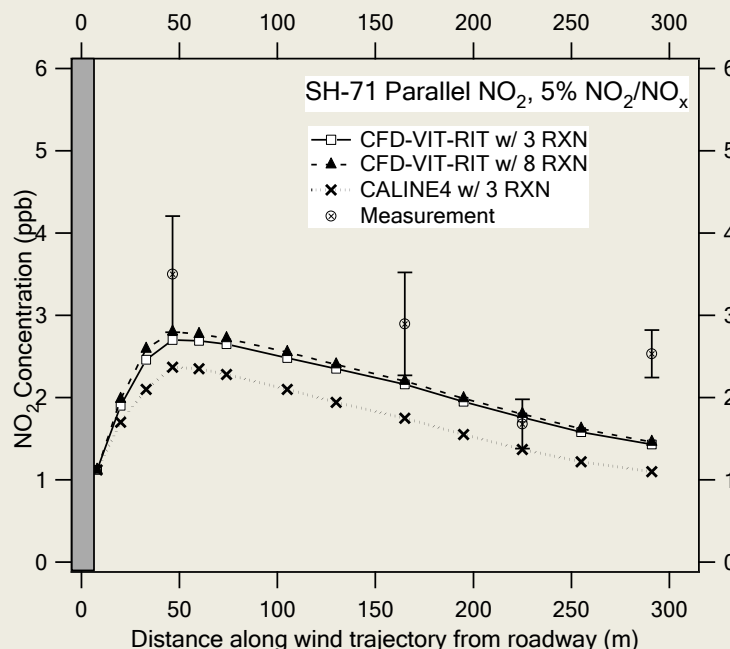
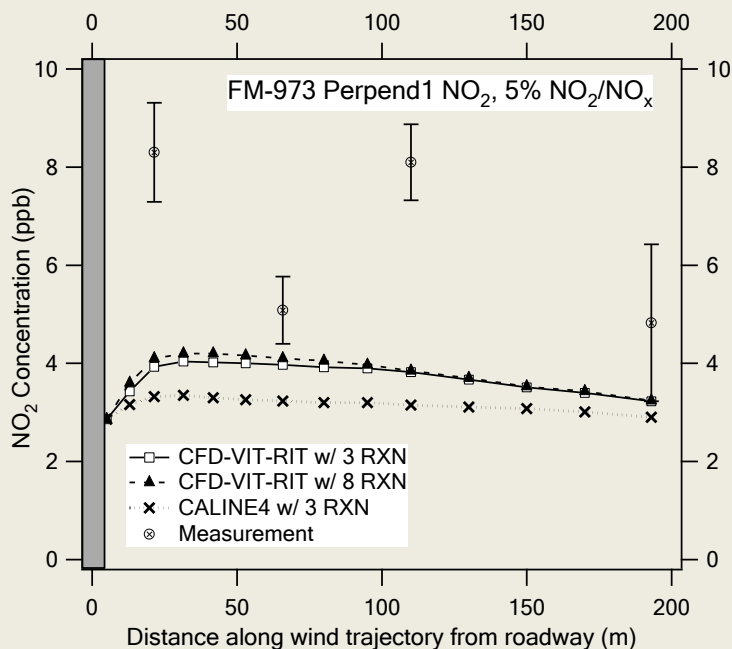
CFD-VIT-RIT: NO_x chemistry near roadways



Highway FM 973 near Austin, TX

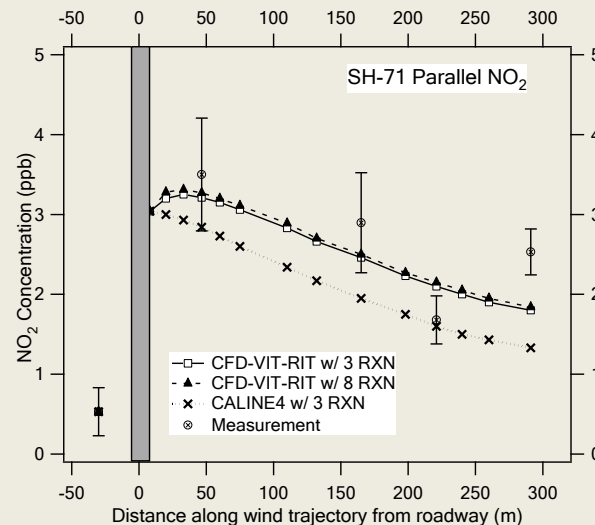
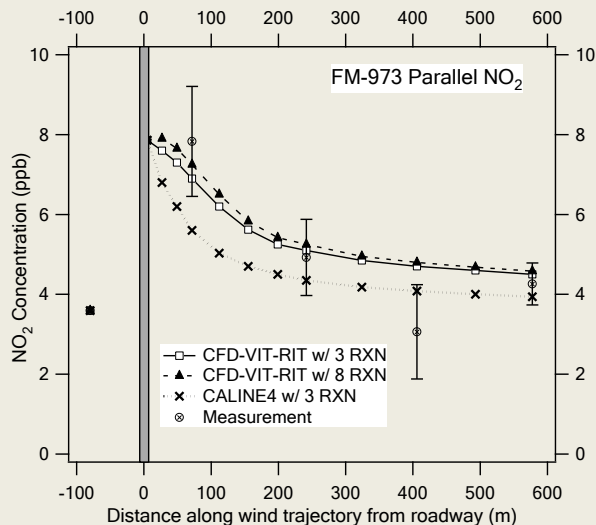
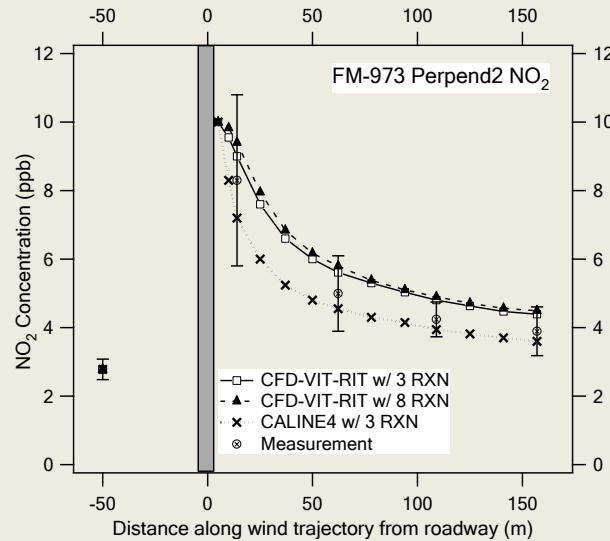
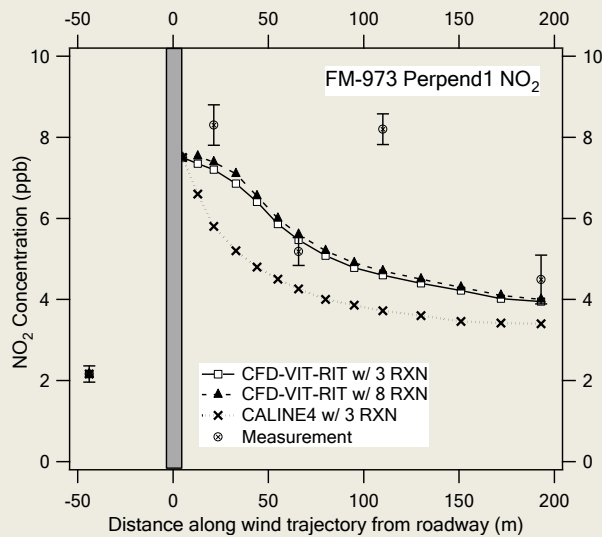
- We applied CFD-VIT-RIT to investigate the chemical evolution of NO_x near Highway FM-973 and SH-71 near Austin, TX.
- The horizontal gradient of NO and NO_x were measured, providing a good dataset for examining the capability of atmospheric models in capturing the chemical transformation of NO₂ near roadways.

NO₂/NO_x Ratio



- Using **5%** NO₂/NO_x ratio, the default value in CALINE4, as the initial condition, neither CFD-VIT-RIT nor CALINE4 can achieve reasonable agreement with the measurement.
- The on-road NO₂/NO_x ratio has changed over time due to several factors including the introduction of aftertreatment devices.
- We extrapolated the curbside NO₂/NO ratios based on measured downwind NO and NO_x concentrations. The NO₂/NO_x ratios ranged from **19 to 31%** for heavy diesel traffic fraction from 5 to 37%.

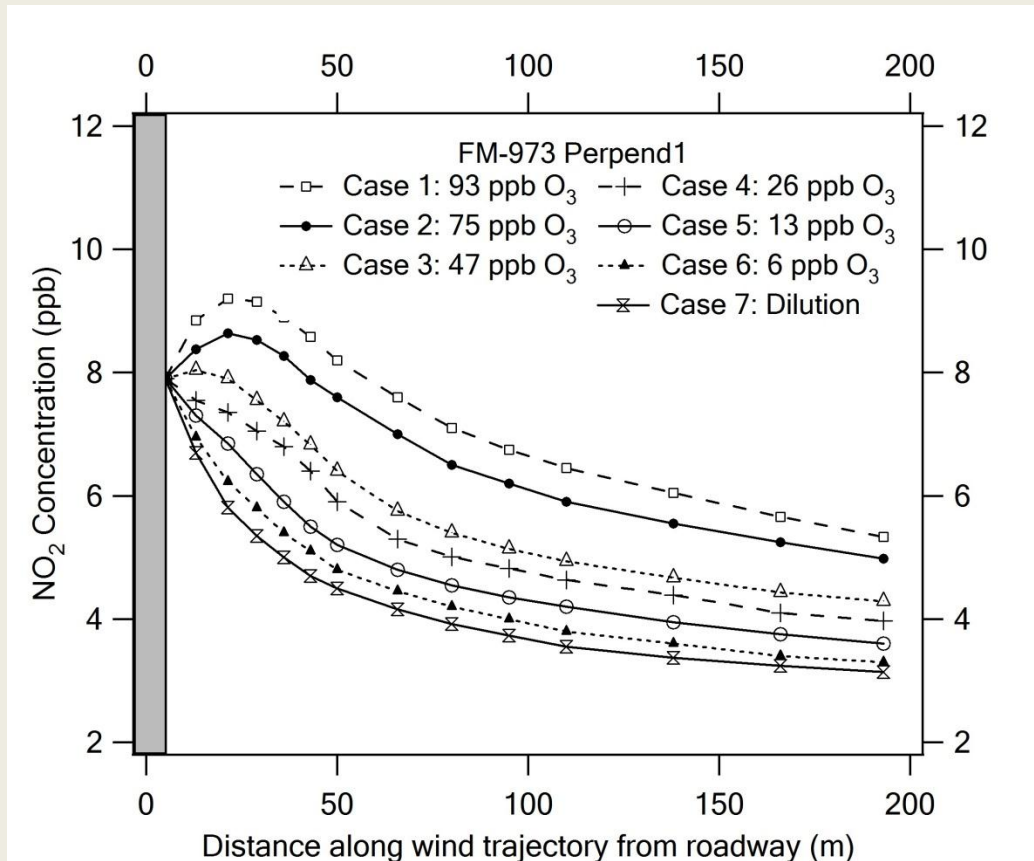
CFD-VIT-RIT: NO_x chemistry near roadways



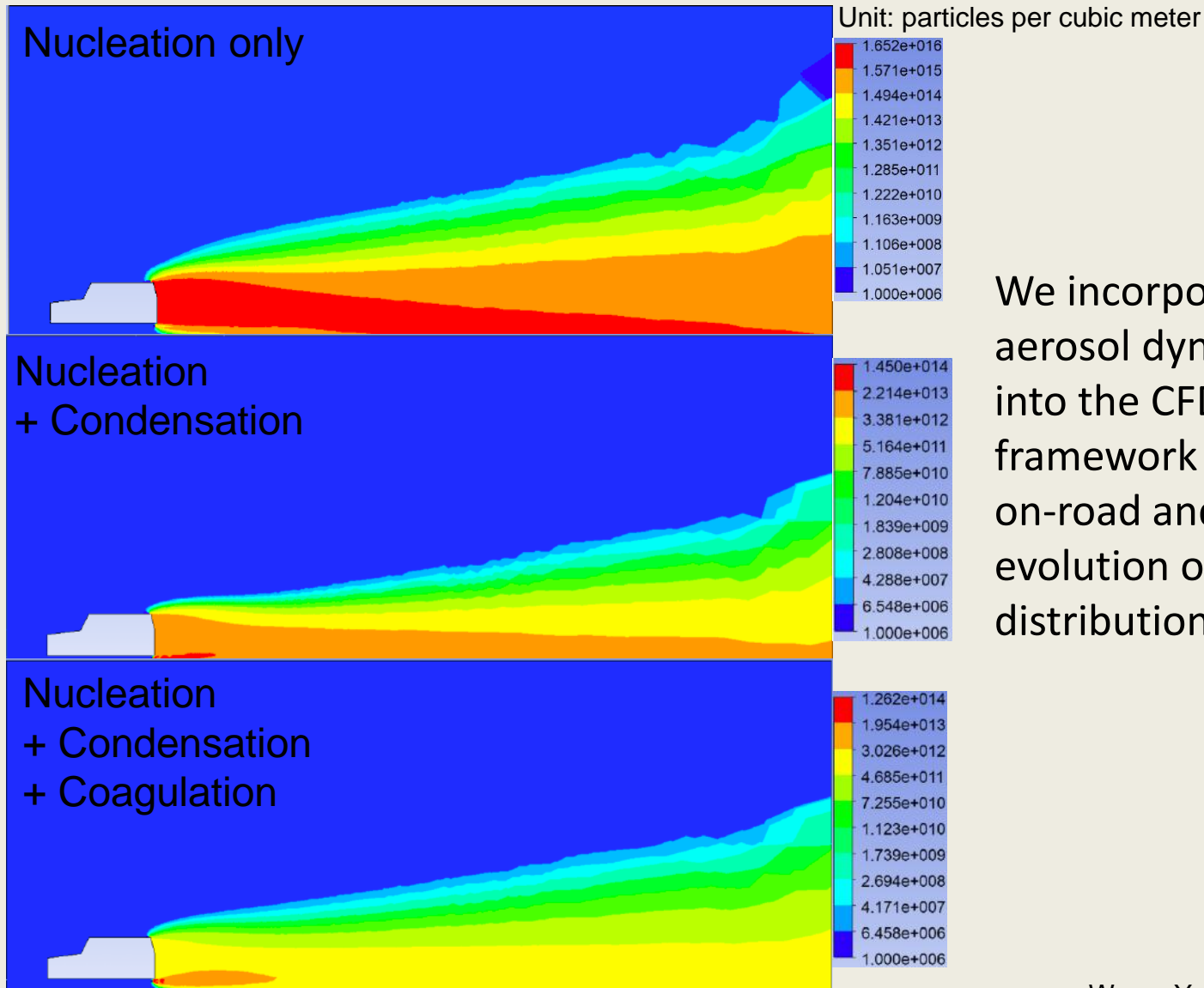
CFD-VIT-RIT couples RANS turbulence model with the finite rate chemical reaction model, which is shown to be capable of predicting both NO_x and NO₂ profiles downwind.

CALINE4 uses a Discrete Parcel Method, which assumes that the NO₂ concentration at a downwind receptor is solely governed by the initial concentrations and time of travel from element to the receptor. *CALINE4 consistently underpredicts NO₂ concentrations.*

CFD-VIT-RIT: NOx chemistry near roadways

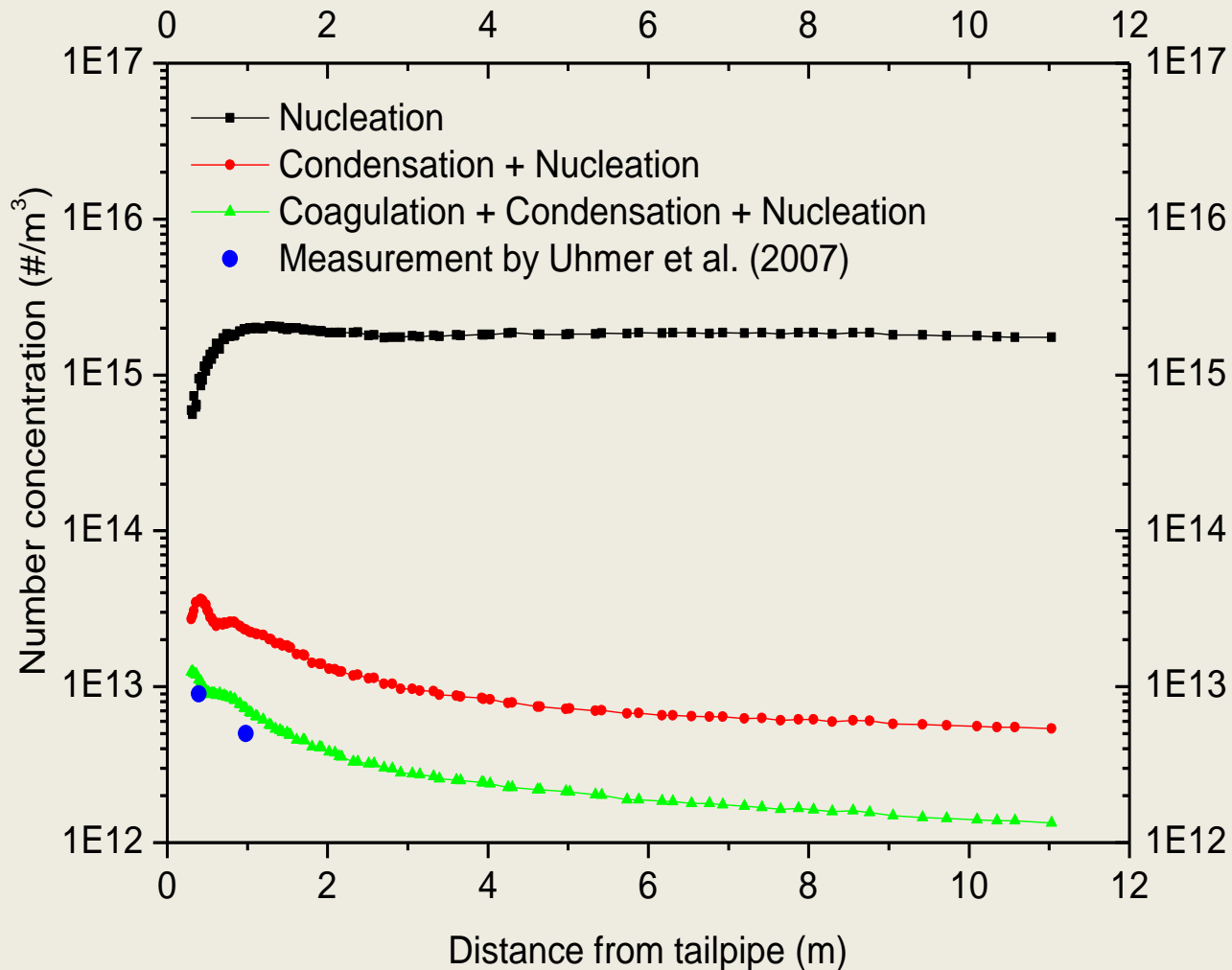


CFD-VIT-RIT: Aerosol dynamics simulation

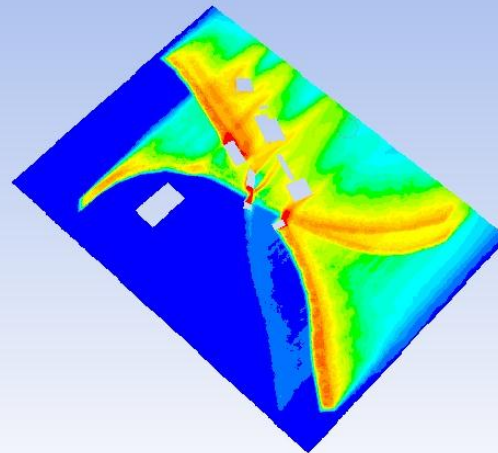
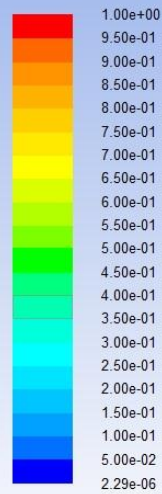
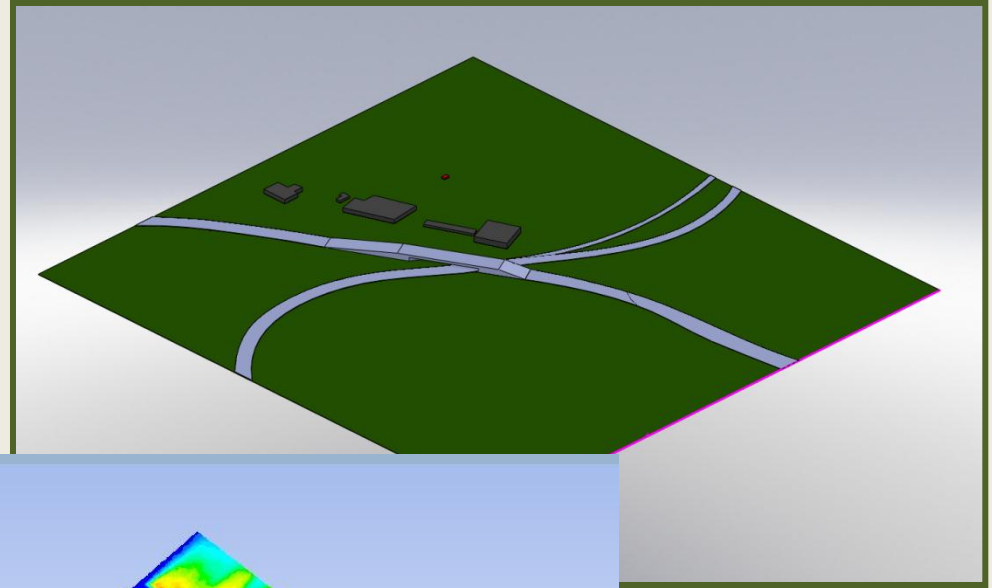
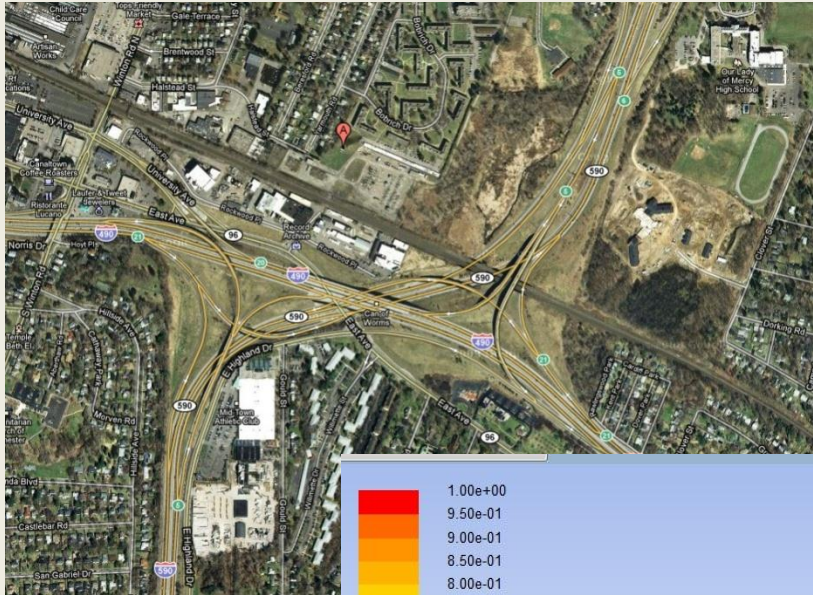


We incorporated a sectional, aerosol dynamics module into the CFD-VIT-RIT framework to simulate the on-road and near-road evolution of particle size distribution.

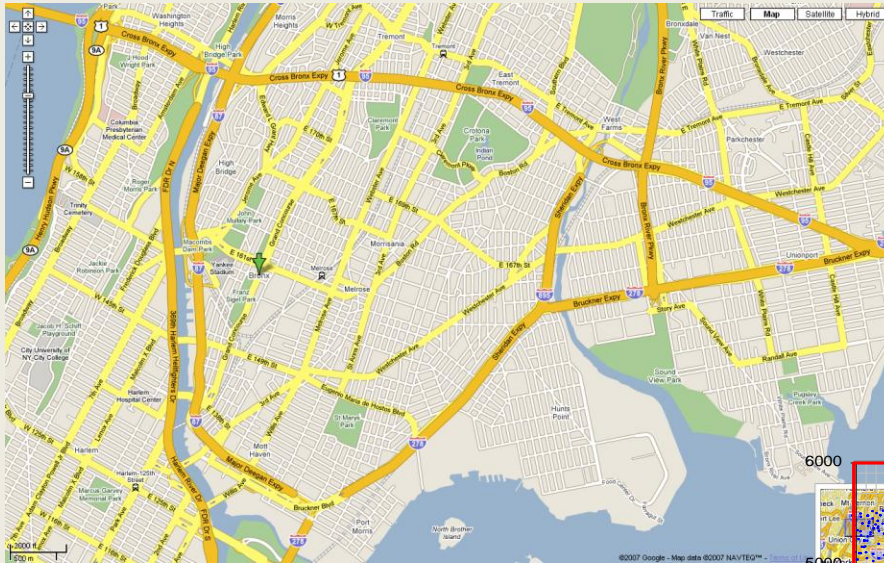
CFD-VIT-RIT: Aerosol dynamics



CFD-VIT-RIT: Pollutant dispersion near highway intersections

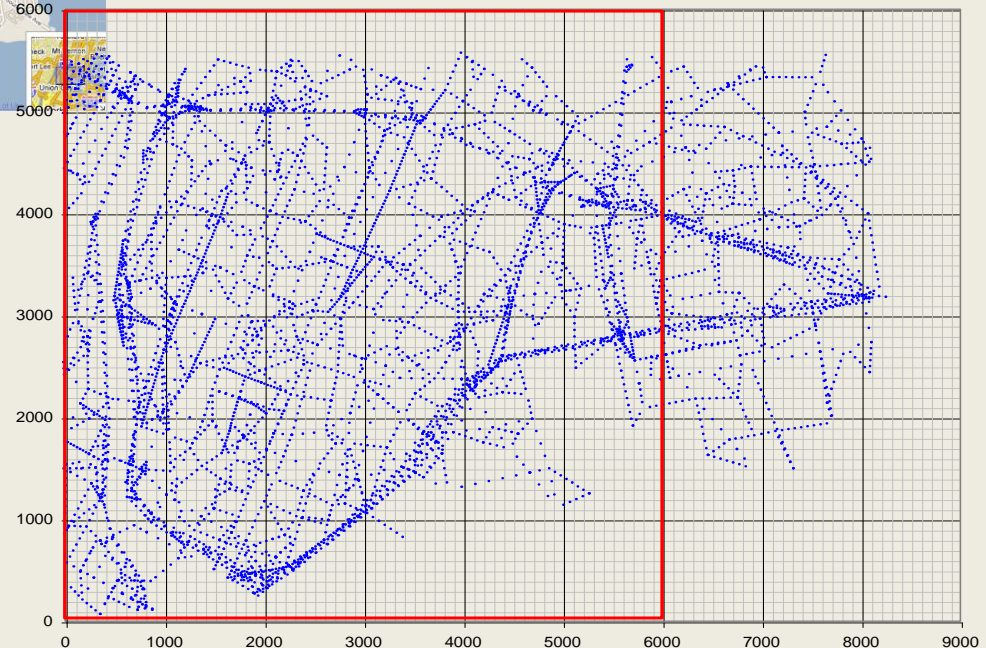


Modeling microenvironment air quality in South Bronx, NYC



- The simulation domain was a 6 km by 6 km area encompassing highways and arterial roads
- Link locations and traffic volume provided by NYMTC
- Emission factors provided by NYSDOT

- The road links were divided to road segments to be modeled as area sources.
- We created over 6,000 road segments for simulation



Simulating Black Carbon Conc. in South Bronx w/ AERMOD

Highest 24-Hr Average BC in March 2004

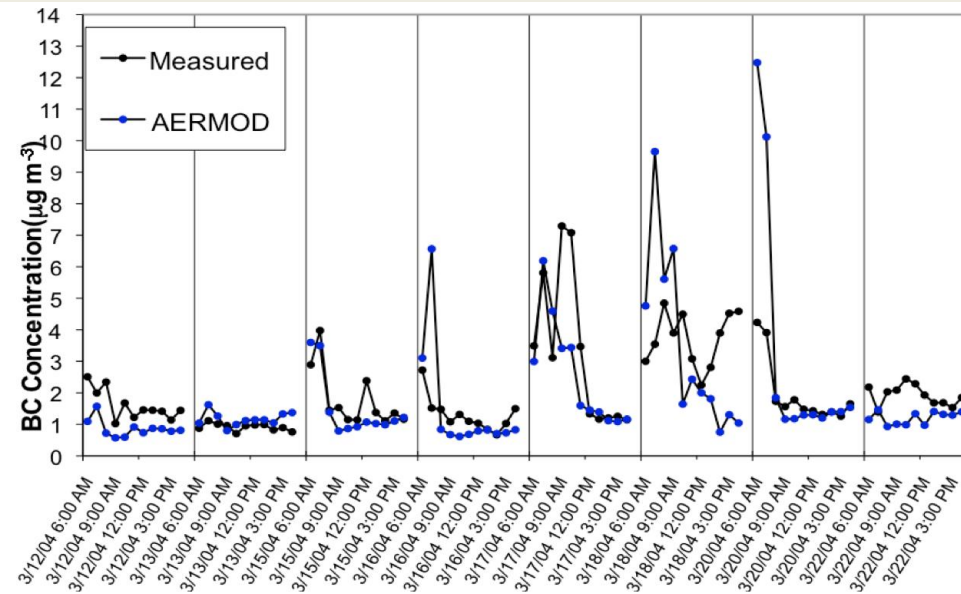
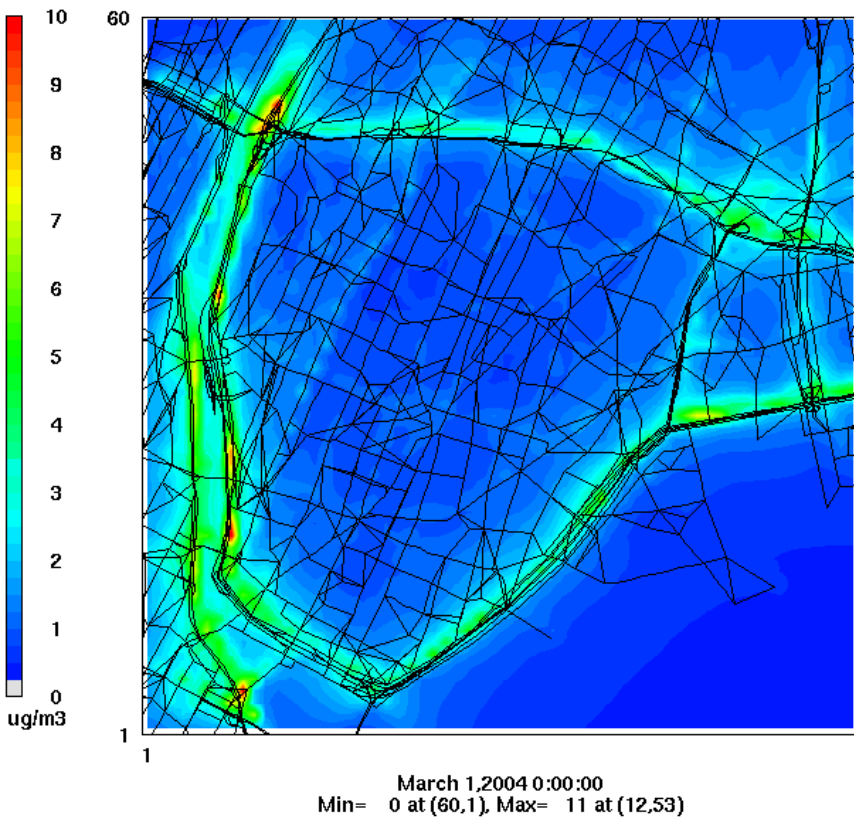


Table 2. AERMOD model evaluation results

<i>Statistical Measures</i>	<i>AERMOD</i>	<i>Accepted Criteria</i>
Mean Normalized Error (MNE)	+40%	+30 to +35% ⁱ
Mean Normalized Bias (MNB)	-6%	±5 to ±15% ⁱ
Unpaired Peak Accuracy (UPA)	+71%	±15 to ±20% ⁱ
Mean Fraction Error (MFE)	+26%	≤ ±75% ⁱⁱ
Mean Fraction Bias (MFB)	-10%	≤ ±60% ⁱⁱ

Discussions

- Turbulent reacting flow models based on computational fluid dynamics (such as CFD-VIT-RIT) have shown great promise in advancing our capability in project-level analysis.
- Those advanced modeling tools are not designed to replace the current Gaussian-based dispersion models. Rather, they can be used to analyze more complex roadway environments, and potentially to be incorporated into highway design processes.
- The caveat is that a CFD model without detailed treatment of atmospheric processes adds no more benefits than the Gaussian models.

Acknowledgment

- EERL students and research associates
- Funding support:
 - New York State Energy Research and Development Authority (NYSERDA)
 - California Air Resources Board (CARB)
 - University Transportation Research Center (UTRC2)
 - Cornell Center for a Sustainable Future

CFD-VIT-RIT: Micro-environment



A complex exposure environment



In a collaborative effort sponsored by the U.S. Federal Highway Administration, regulators, researchers, and consultants identify and prioritize research needs for the transportation community.

PARTICULATE MATTER: A Strategic Vision for Transportation- Related Research

MICHAEL C. McCARTHY
DOUGLAS S. EISINGER
HILARY R. HAFNER
LYLE R. CHINKIN
PAUL T. ROBERTS
SONOMA TECHNOLOGY, INC.
KEVIN N. BLACK
U.S. FEDERAL HIGHWAY ADMINISTRATION
NIGEL N. CLARK
WEST VIRGINIA UNIVERSITY
PETER H. McMURRY
UNIVERSITY OF MINNESOTA
ARTHUR M. WINER
UNIVERSITY OF CALIFORNIA, LOS ANGELES

Most individuals have witnessed a bus or large truck emitting a thick smoke plume as it accelerates away from an intersection. Or they have seen the occasional car trailing a smoke cloud in its wake. When cars and trucks emit visible smoke, their contribution to air pollution is obvious. However, on-road vehicles, or "mobile sources", emit a range of pollution. Some pollutants, such as carbon monoxide (CO) and soot from diesel-powered trucks, are emitted straight from the tailpipe. Other vehicle emissions, like volatile organic compounds (VOCs), NO_x, and ammonia, interact in the atmosphere to form "secondary" pollutants, such as ozone or ammonium nitrate.

PHOTO: SC