Numerical and statistical analyses in sustainable energy and transportation

Anirban Roy

18th November, 2019

MY RESEARCH SUMMARY

Mathematical modeling

Numerical modeling	Statistical modeling
3-D regional air quality modeling (a.k.a chemical transport modeling or photochemical grid modeling) Vehicle energy consumption in multiple modes	Markov chain Monte Carlo modeling of plug flow reactor

Data analysis

Uncertainty quantification	Big data analysis
e.g. estimating uncertainty in combusiton emissions and identifying corresponding drivers	e.g. identifying emissions and energy consumption patterns using on-board diagnostics

MODELING AND SIMULATION STUDIES

Study	Execution	Institute
Simulation of titania nanoparticle nucleation, coagulation and finite rate sintering in an externally heated plug flow reactor using a Monte Carlo method	MTech	IITK
Modeling source marker depletion in the atmosphere and its implication for receptor modeling	PhD	CMU
Modeling the air quality impacts of Marcellus Shale gas development	PhD	CMU
Air quality changes of motor vehicle electrification over the Houston metropolitan area	Post-doc	UH
Simulation of energy consumption in varying load-RPM bins for off-road construction equipment	Research scientist	CARB

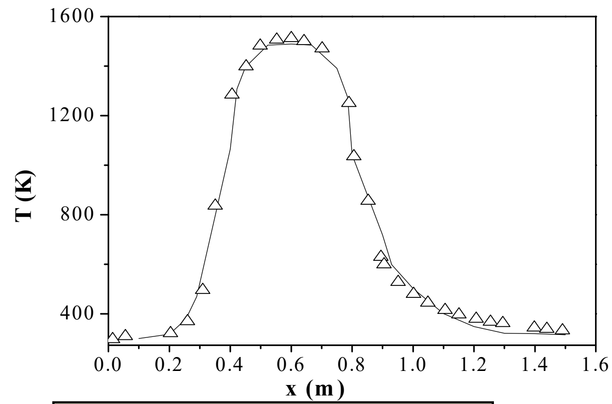
DATA ANALYSIS STUDIES

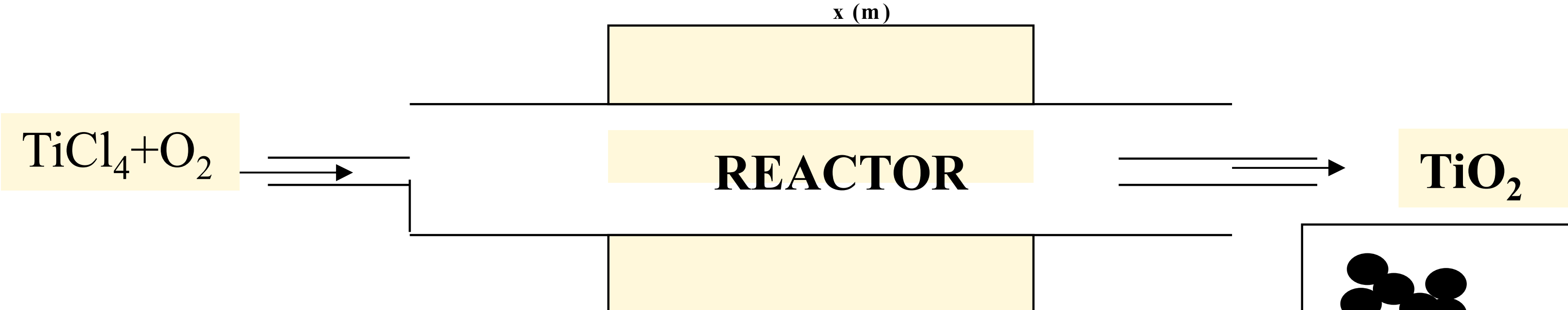
Study	Execution	Institute
Constructing an emissions inventory for unconventional natural gas development in the Marcellus Shale and estimating the uncertainty therein	PhD	CMU
Evaluating the effects of temperature and driving conditions on gasoline exhaust VOC speciation	Post-doc	UH
Developing a 2-D framework to assess emissions from construction equipment as a function of engine load and RPM	Research Scientist	CARB

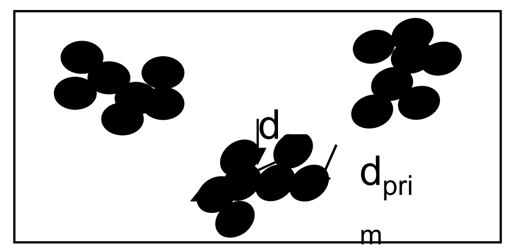
Titanium dioxide (titania/TiO_2)

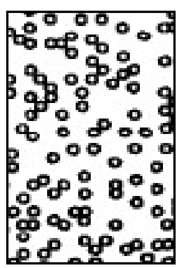
- Applications in cosmetics and photochemical wastewater treatment
- Recent applications: anode material in Li-ion batteries as 3-D intercalation material (LTO)
- Formation through aerosol routes - no need for consequent separation as opposed to solution method.

Modeling titania formation

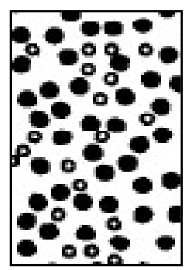








Condensible molecules



Nucleation [1]

Coagulation and subsequent finite sintering. to form dendritic, fractal aggregates [§]**.**

[1] ***After Panda and Pratsinis (1995)***

§ ***After Kataria(2006)***

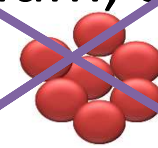
Nucleation

Titania nanoparticles

- Critical cluster size ~ 1 molecule

~~Metal nanoparticles~~

~~e.g. indium, aluminum~~



- ~~Critical cluster size > 1 molecule~~

- Hence, reaction ~ nucleation for TiO_2.

Reaction rate constants

- **Pratsinis et al., 1990:**
- $\frac{d[TiCl_4]}{dt} = \left(k_A + k_B[O_2]^{\frac{1}{2}}\right)[TiCl_4]$
- $k_A = 8.26 \times 10^4 \, e^{-\frac{E_A}{RT}} \, s^{-1}$, *rate constant for* $TiCl_4$
- $k_B = 1.4 \times 10^4 \, e^{-\frac{E_A}{RT}} \, (L/mol)^{1/2} s^{-1}$, *rate constant for* O_2,
- $E_A = E_B = 88 \, J \, mol^{-1}$, *activation energy for both rate constants*

- Moody and Collins, 2003:
- $\frac{d[TiCl_4]}{dt} = (k_A + k_B[O_2])[TiCl_4]$
- $k_A = 4.1 \times 10^4 \, e^{-\frac{E_A}{RT}} \, s^{-1}$, *rate constant for* $TiCl_4$
- $k_B = 4.8 \times 10^8 \, e^{-\frac{E_A}{RT}} \, Lmol^{-1}s^{-1}$, *rate constant for* O_2
- $E_A = 91 \, J \, mol^{-1}$, $E_B = 107 \, J \, mol^{-1}$

Coagulation

Particles of a given volume v being born due to aggregation between smaller particles

$$B_{agg} = (1/2)\int_0^{\infty} \beta_{v',v-v'} n(v')n(v-v')dv'$$

Particles of a given volume v dying due to aggregation with the entire particle size range

$$D_{agg} = n(v)*\int_0^{\infty} \beta_{v,v'} n(v')dv'$$

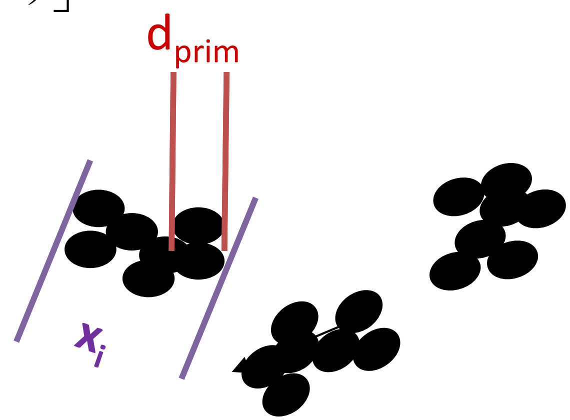
Coagulation kernel between particles of two different sizes

$$\beta_{v_i,v_j} = 2\pi(D_i+D_j)(x_i+x_j)\left[\left(\frac{x_i+x_j}{x_i+x_j+2g_{ij}}\right)+8\left(\frac{D_i+D_j}{c_{ij}(x_i+x_j)}\right)\right]^{-1}$$

Aggregate particle diffusivity

Aggregate particle diameter (accounting for fractal shape)

$$x_i = d_{prim}\frac{v_i}{v_{prim}}^{\frac{1}{D_f}}$$



Finite rate sintering

- Finite sintering in ceramics (unlike instantaneous in metals).
- $$d_{prim,t+\Delta t} = d_{prim,t} + \frac{d_{prim,t}\left(1-(K+1)^{-\frac{1}{3}}\right)}{t_f}\Delta \mathrm{t}$$
- K = coordination number (how many particles surround one primary particle), t_f = sintering time.

Gas-phase sintering mechanisms

Grain boundary diffusion

$$t_f = \frac{0.013 k_B T d_{prim}{}^4}{16 w D_{gb} \sigma v_o}$$

Grain boundary diffusivity

Grain boundary width

Lattice diffusion

$$t_f = \frac{RT d_{prim}{}^3}{128 D_l \sigma v_o}$$

Lattice diffusivity

Time scales and fractal dimension

Coordination number

$$K = K_{min} + \frac{D_f - D_{f,min}(K_{max} - K_{min})}{D_{f,max} - D_{f,min}}$$

Fractal dimension

$$D_f = \left\{ D_{f,min} + (D_{f,0} - D_{f,min})^{\frac{1}{\tau^s}} \right\} \tau \le 1$$

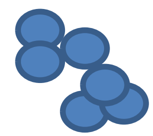
$$= \left\{ D_{f,max} - (D_{f,max} - D_{f,0})^{\tau^s} \right\} \tau > 1$$

$$D_{f,max} = 3, D_{f,min} = 1.7, \ D_{f,0} = 2.35$$

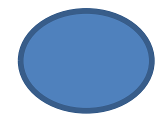
$$\tau = \frac{t_c}{t_f} = \frac{\text{Time elapsed between consecutive collisions}}{\text{Time required for complete sintering}}$$

Two limiting cases

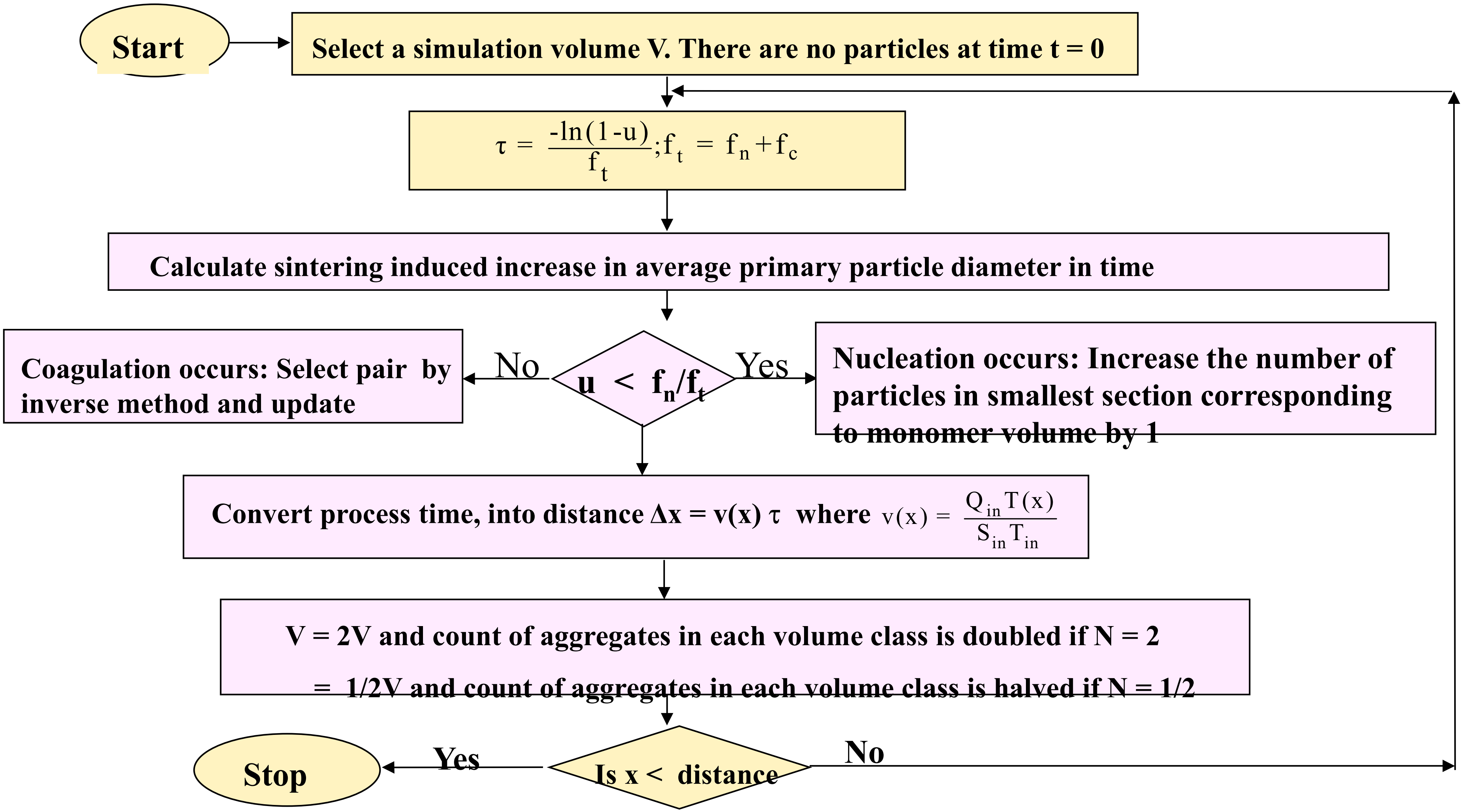
τ<<1



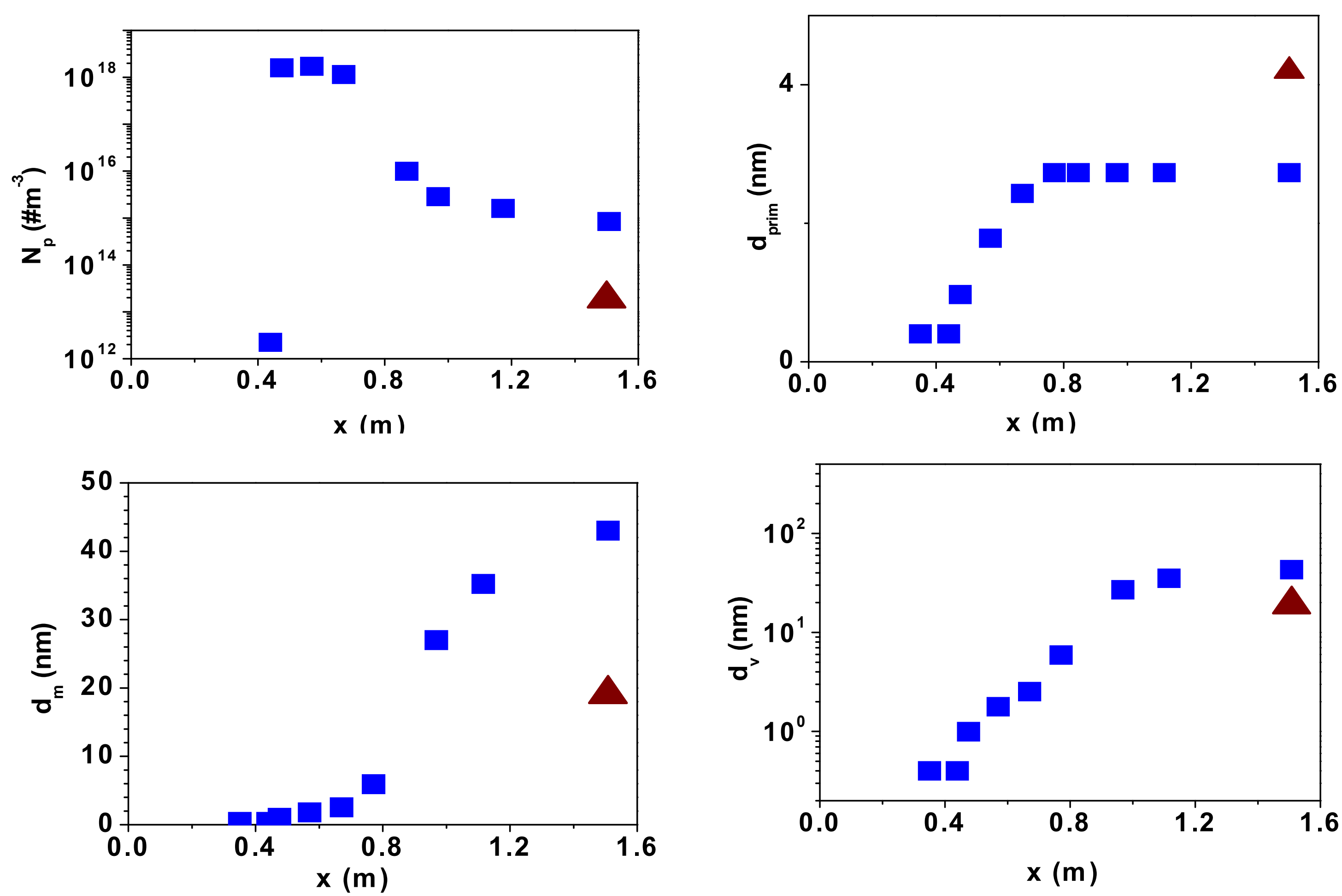
T>>1



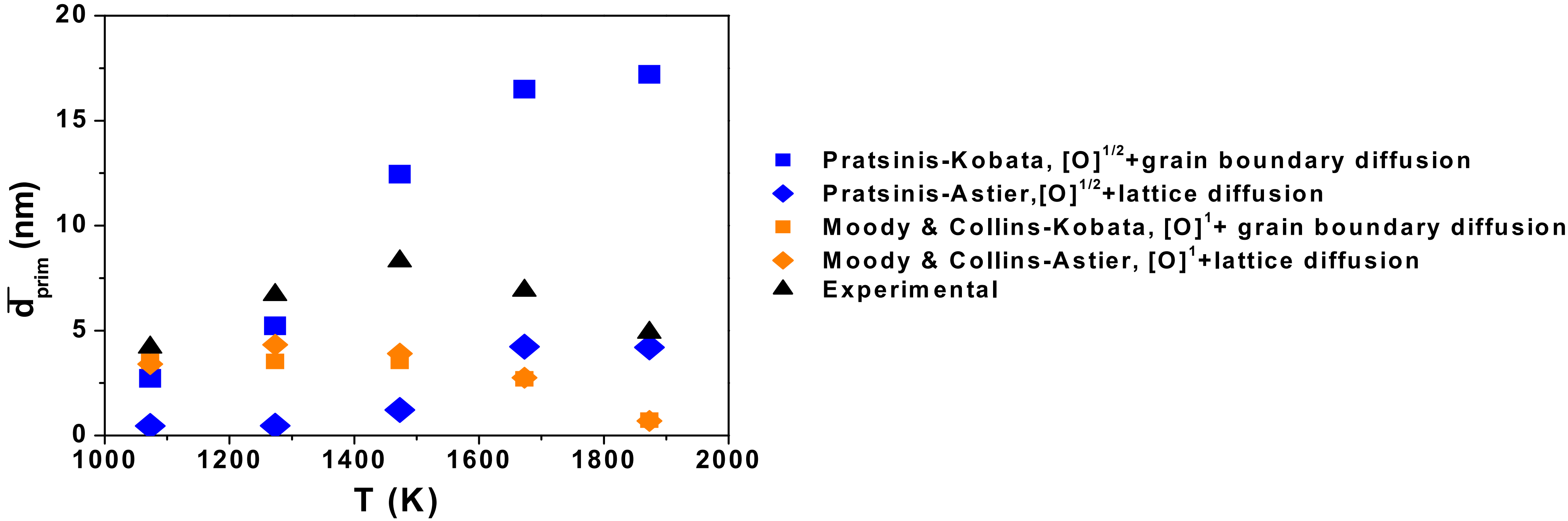
The Simulation Algorithm



Evolution of Aerosol Characteristics: 1073K

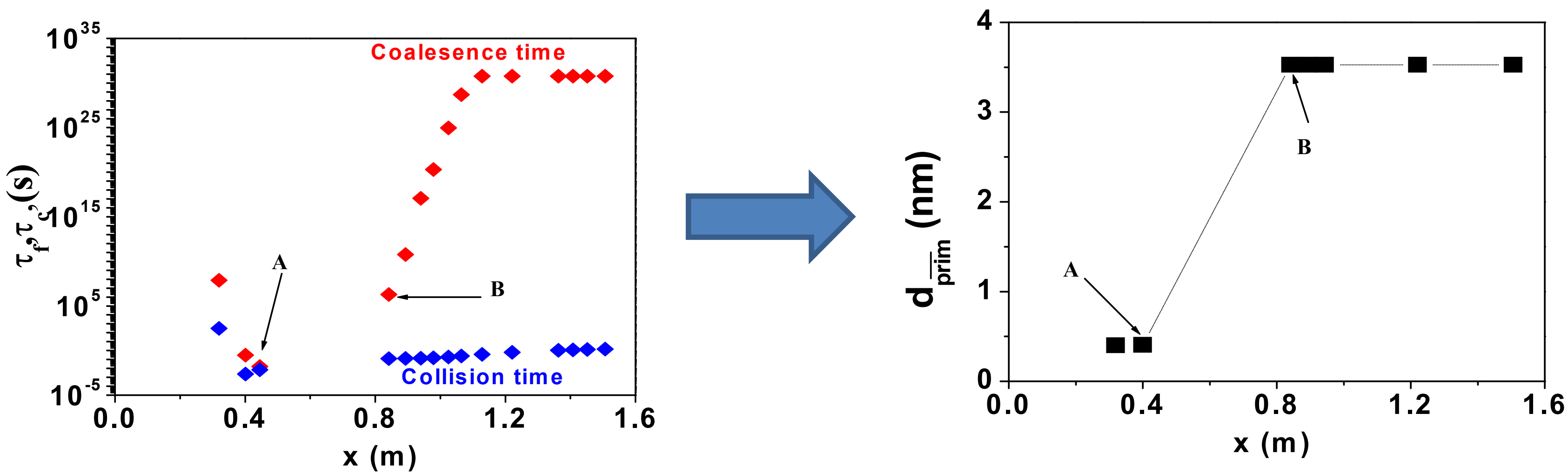


Model-measurement evaluation



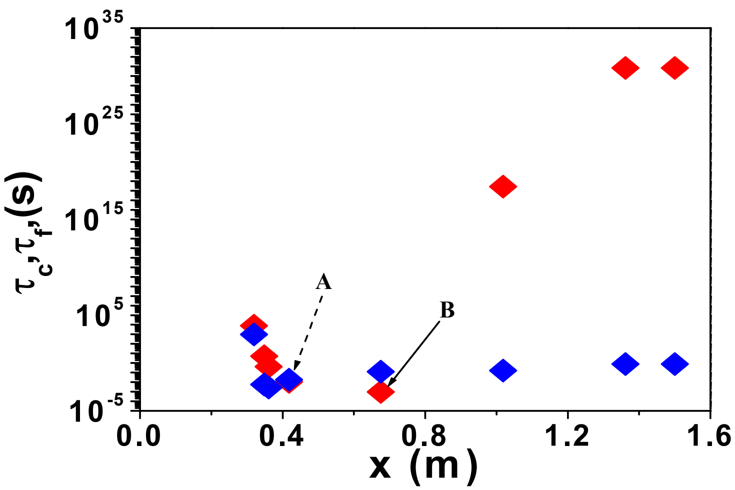
- Primary particle diameter as case study – other parameters (particle number density, volume and surface area equivalent diameter showed similar trends).
- At low temperatures, use of rate constant first order in oxygen, and grain boundary diffusivity in sintering gave better model performance.
- At higher temperatures, rate constant half-order in oxygen, with lattice diffusion in sintering gave better performance.

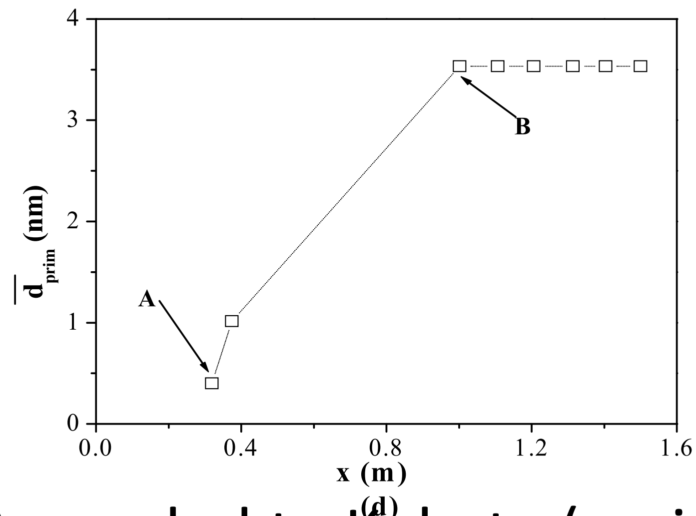
Spatial evolution of collision and coalescence time scales and implications to sintering : Pattern 1



- Moody Collins rate expression ($[O]^1$) coupled to Kobata (grain boundary diffusion sintering), 1073K
- Sintering immediately freezes leading to early saturation of primary particle diameter

Spatial evolution of collision and coalescence time scales and implications to sintering : Pattern 2





- Moody Collins rate expression ([O]^1) coupled to Kobata (grain boundary diffusion sintering), 1073K
- We see a zone where collision and coalescence time scales overlap.
- This ensures sintering continues over a greater reactor length

Conclusions

- A stochastic Monte Carlo algorithm was developed and extended to simulate the formation of TiO_2 nanoparticle synthesis in an externally heated plug flow reactor.
- Two reaction mechanisms (first and half order wrt oxygen) and two sintering mechanisms (grain boundary and lattice diffusion) were tested at 5 maximum reactor temperatures: 1073K, 1273K, 1473K, 1673K and 1873K.
- For T<1473K, a combination of reaction rate 1st order in oxygen and grain boundary diffusion for sintering gave better model-measurement performance.
- A combination of reaction rate half-order in oxygen and lattice diffusion gave better performance at higher reactor temperatures.
- Two spatial evolution patterns of sintering and collision times were found – that dictated the onset of freezing primary particle diameter.

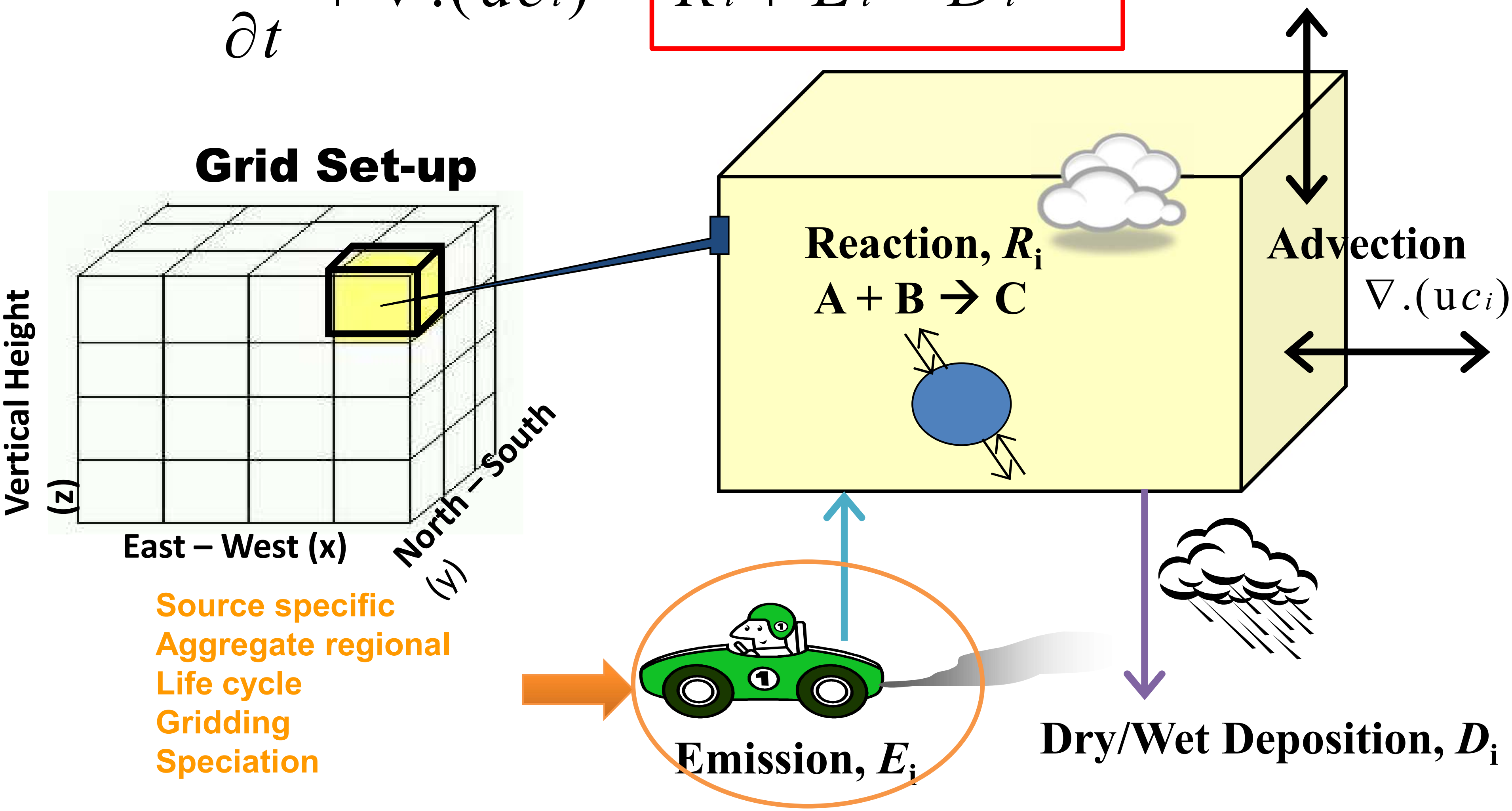
Chemical transport modeling

	Chemical/metallurgical/mechanical engineering systems	Atmospheric systems
What is discretized into x, y and z- grid cells?	e.g. plug flow reactor blast furnace IC engine	state/country/entire globe
Grid cell size	< 1 mm	1 km – 100 km
Time scales	10^{-6} -1 s	10^{-9} s to several decades
Species simulated	<10?	100-500

PMCAMx : The chemical transport model

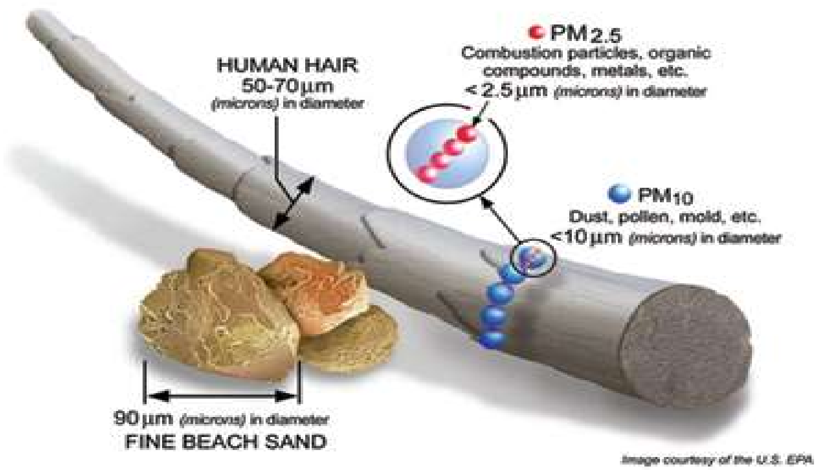
$$\frac{\partial c_i}{\partial t} + \nabla.(\mathrm{u}c_i) = \boxed{R_i + E_i - D_i}$$

Model forcing functions



Particulate matter, PM2.5

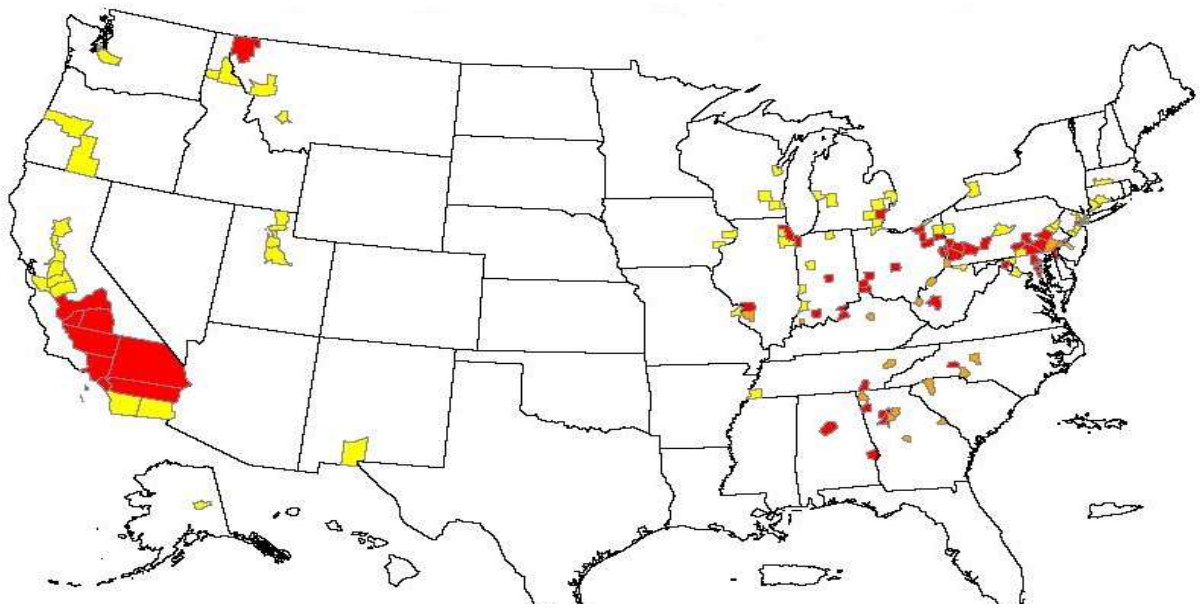
Size in context



Recent smog episode in Beijing

- High concentrations →increased mortality, morbidity, pulmonary damage.
- Affects climate change.

Status of fine particle pollution in the US



Both annual (15 µg $^{-3}$) and 24-hr(35 µg m^{-3}) standard

ONLY the 24-hr (35 µg m^{-3}) standard

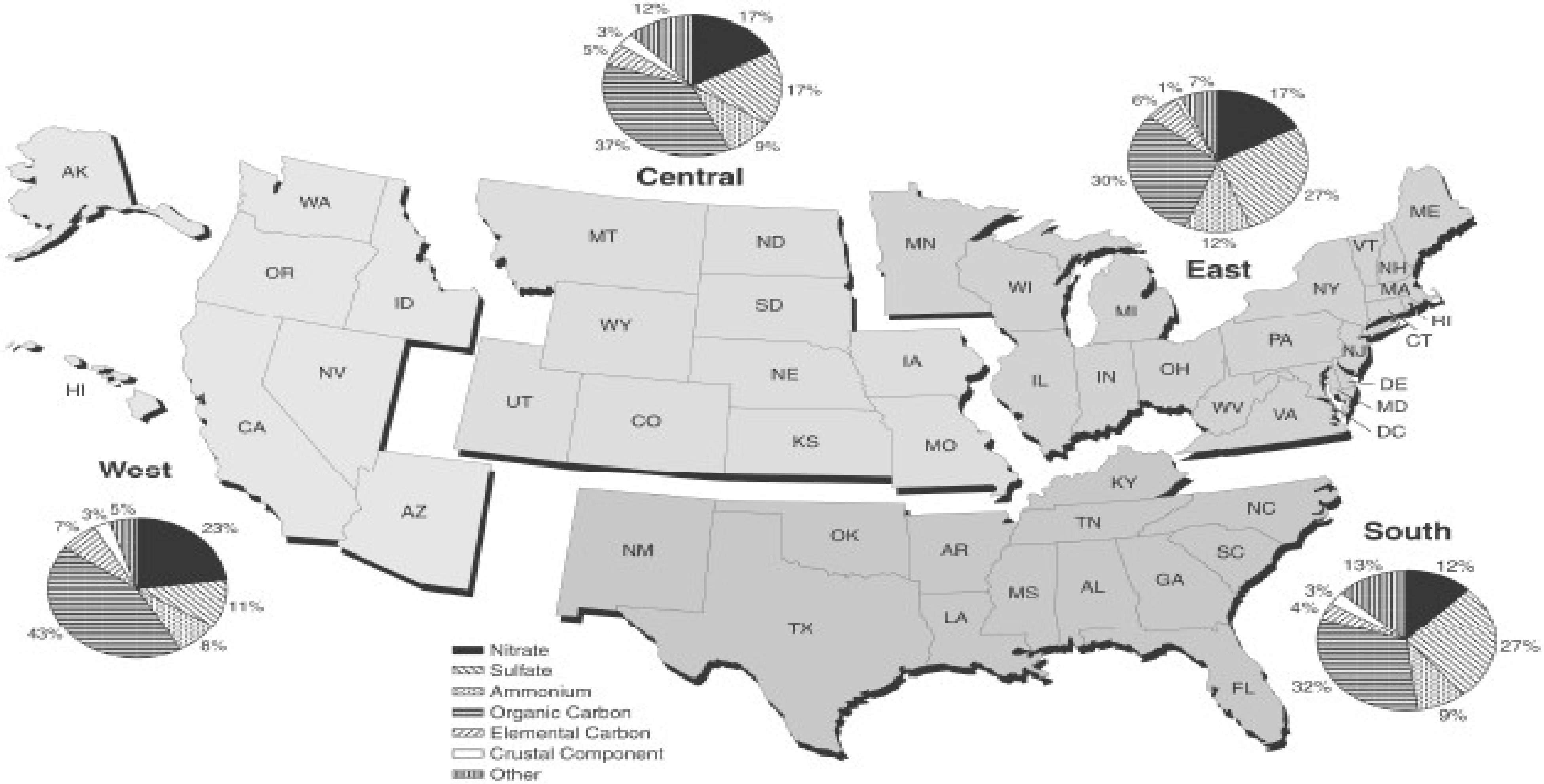
ONLY the annual (15 µg m^{-3}) standard

~ 90M Americans live in areas that violate annual PM standard

http://www.epa.gov/air/oaqps/greenbook/qnsum.html

http://www.epa.gov/oar/particlepollution/naaqsrev2006.html#maps

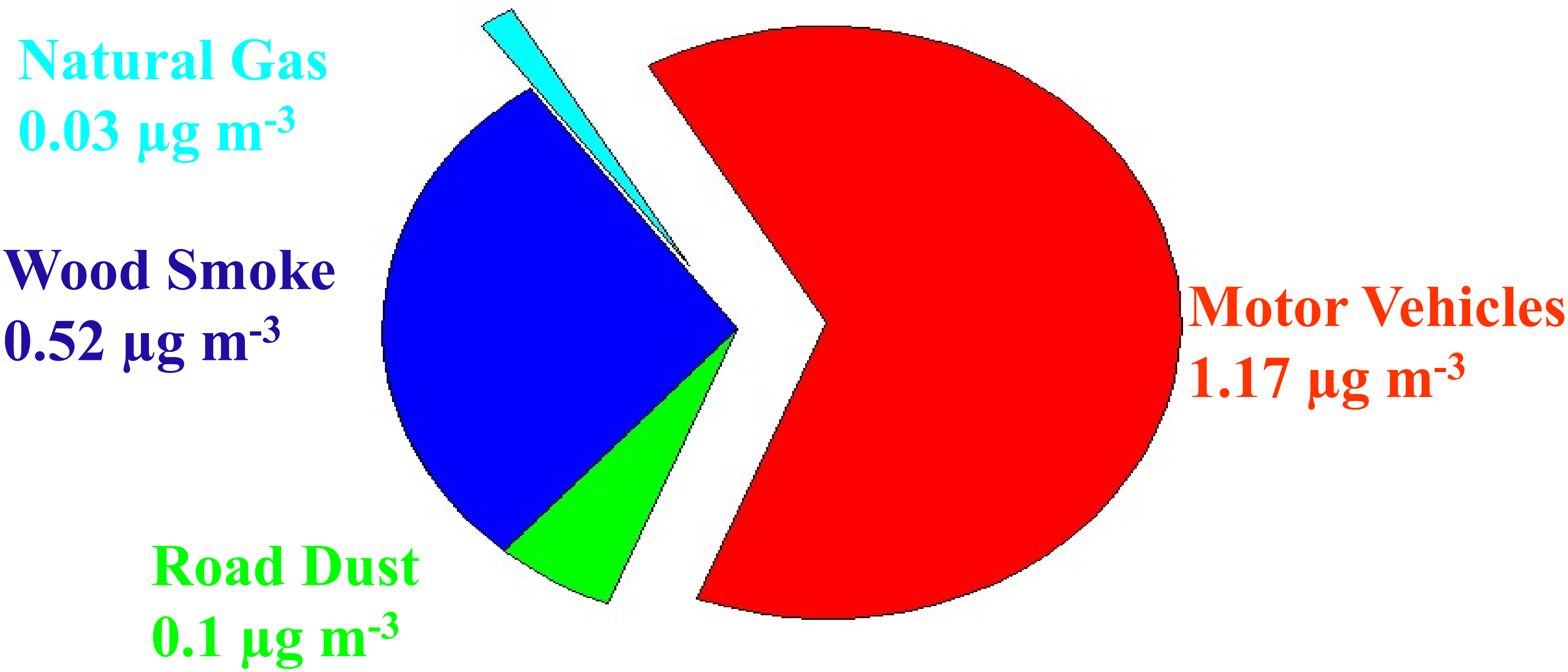
Speciated components of PM2.5



- Organic carbon (OC) occupies a significant fraction

Jayanty et al., 2002

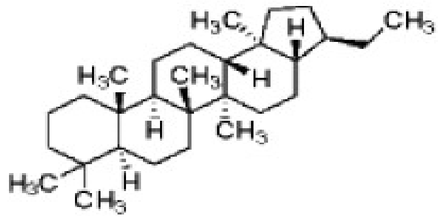
Source apportionment of primary particulate matter



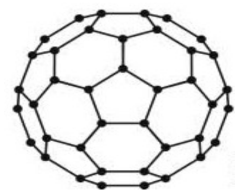
Zheng et al., 2001

Molecular markers

Norhopane



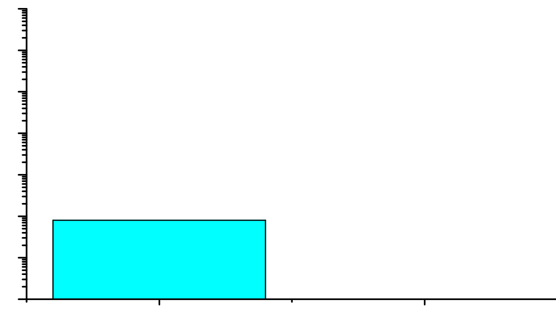
Elemental Carbon



- Species used to fingerprint source influences
- Assumed photochemically stable in atmosphere (~ “tie” material in process calculations)
- Norhopane (a polycyclic alkane) fingerprints gasoline exhaust OC emissions
- Elemental carbon (buckyball) fingerprints diesel OC emissions

Receptor model for norhopane

Ambient Concentrations (C_i)



=

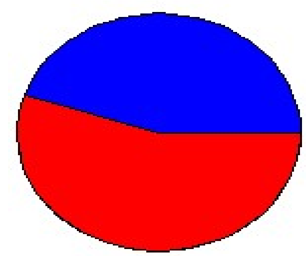
Norhopane (Gasoline)

+

Norhopane (Diesel)

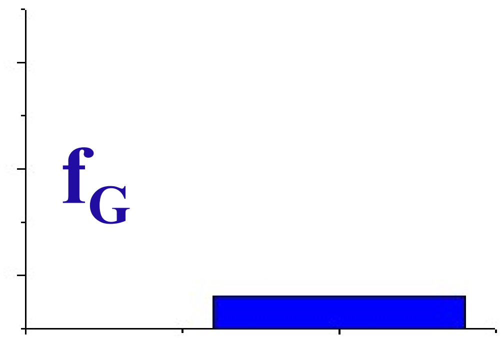
=

Source Contributions (G, D)



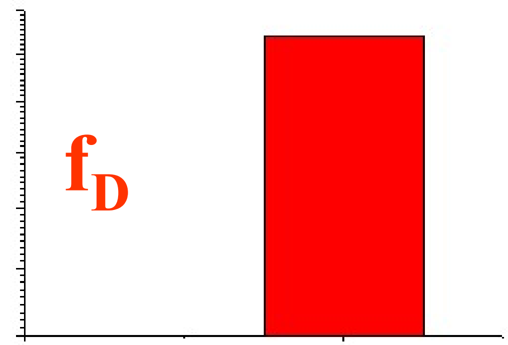
Fractional content in source

$G \times f_G$



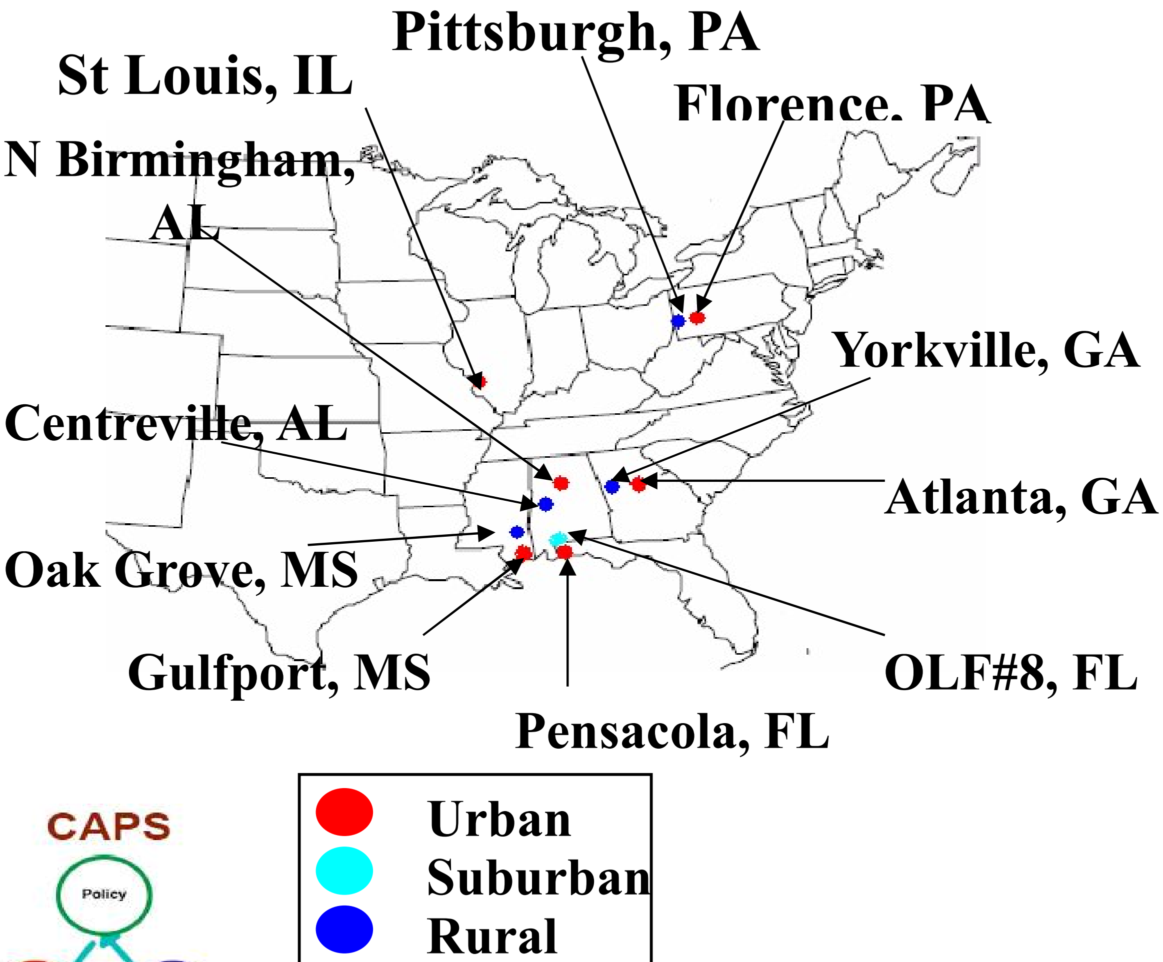
+

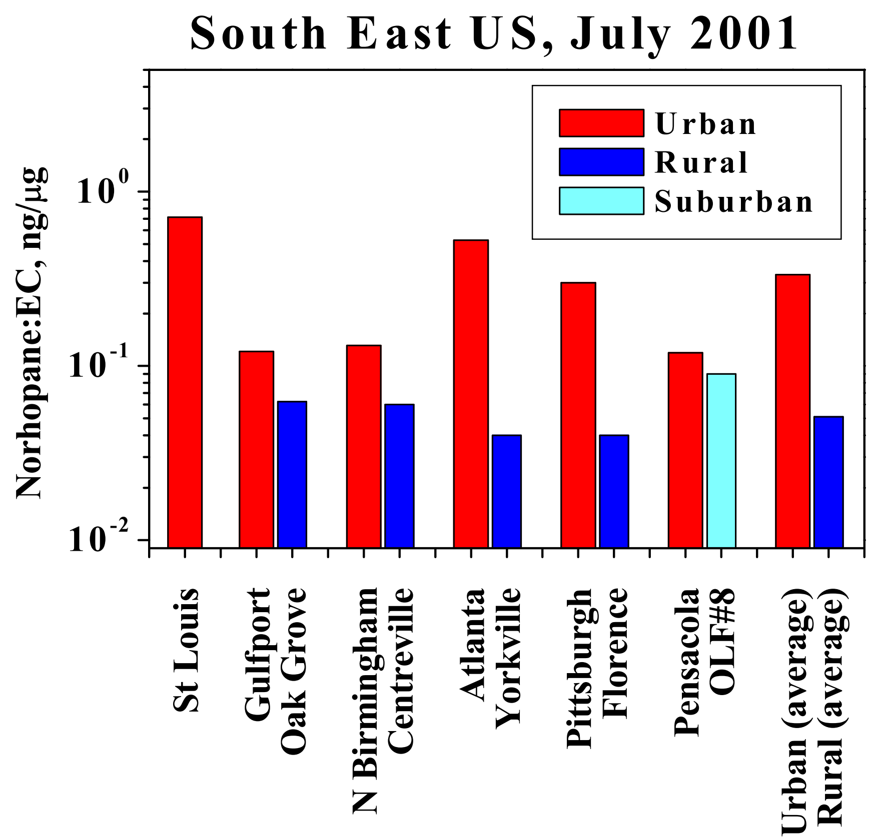
$D \times f_D$



These models assume tracers to be nonreactive

What do field data say?

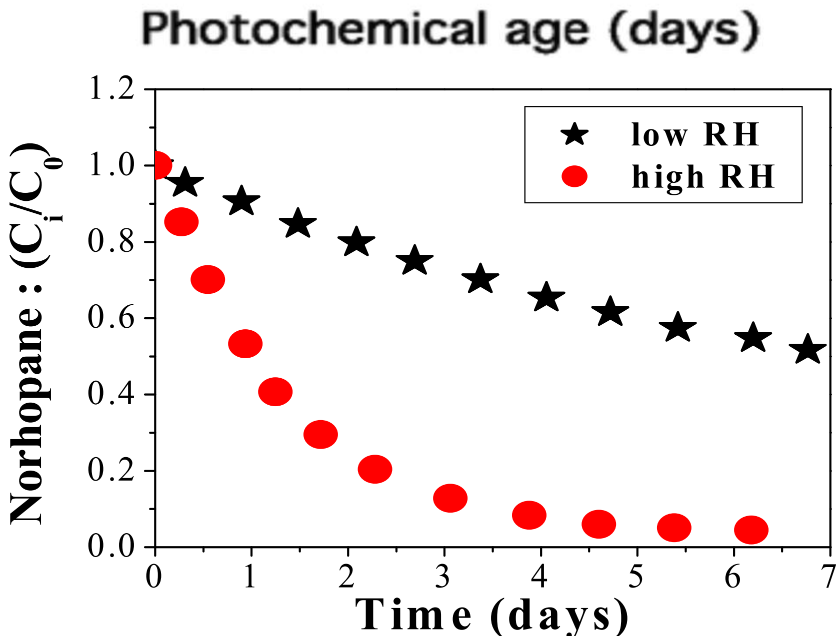




CAPS
Policy
Science
Engineering
Carnegie Mellon

Robinson et al., 2006
Zheng et al., 2002

What do laboratory data say?



Lambe et al., 2009
Weitkamp et al., 2008

- Smog chamber studies: basically a well-mixed box made of teflon
- Norhopane injected in various chemical matrices – e.g. motor oil, diesel exhaust; reacted with OH radical produced photochemically in the presence of UV radiation. Samples withdrawn at regular intervals
- Upto 60% reduction in ~ 1 day which is the typical residence time (akin to space time in reactors) of an air mass in an urban region.

Key questions

- What is
  - the fraction of Norhopane reacting regionally?
  - the resulting bias motor vehicle OC?
  - the bias in the gasoline-diesel split?

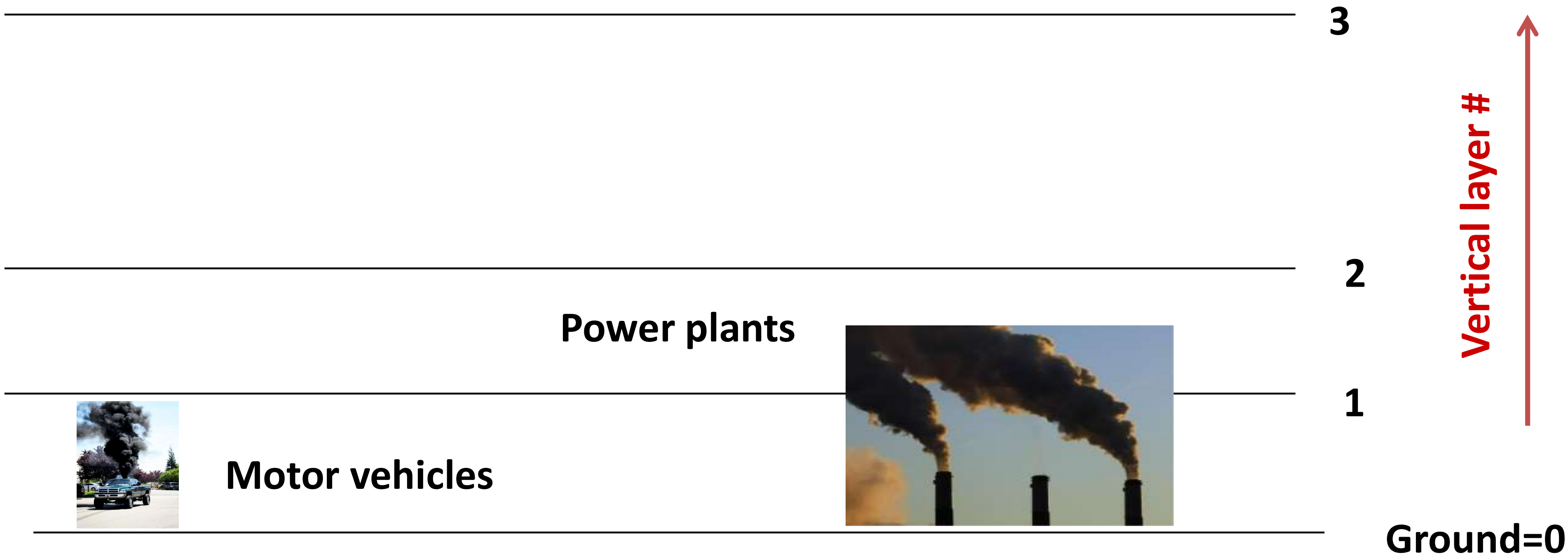
We modified an existing Chemical Transport Model (PMCAMx) to answer the above questions.

Key extensions to model: Norhopane emissions

- Norhopane source term as a forcing function

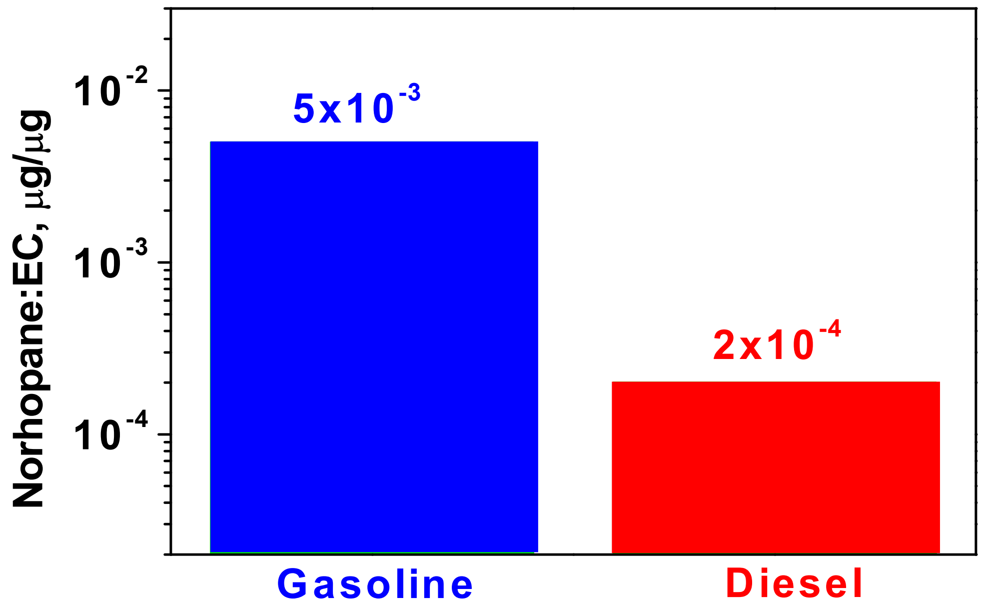
$$\left(\frac{[Norhopane]}{[EC]}\right)_{Gasoline} \times E_{EC,Gasoline} + \left(\frac{[Norhopane]}{[EC]}\right)_{Diesel} \times E_{EC,Diesel} = E_{Norhopane,total}$$

Area vs point sources



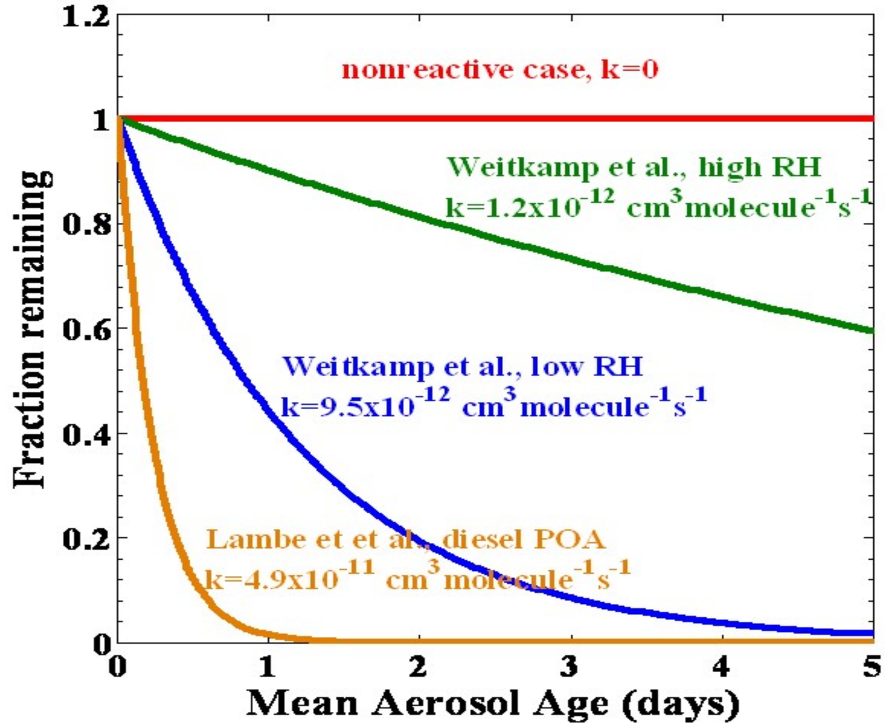
- Area sources emit within the first vertical layer. Others are classified as point sources.
- Point sources also have a plume velocity, temperature and plume height rise

Norhopane-to-EC ratios



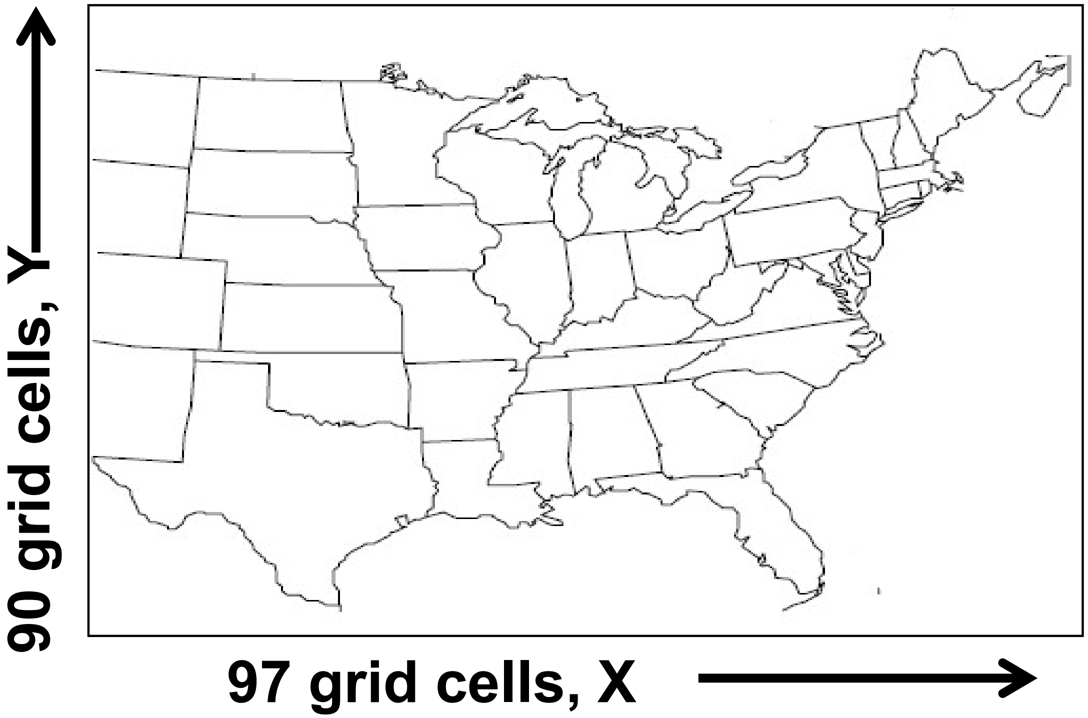
- Experimentally obtained from vehicle emissions tests where an urban drive cycle is simulated in a lab

Reactivity scenarios



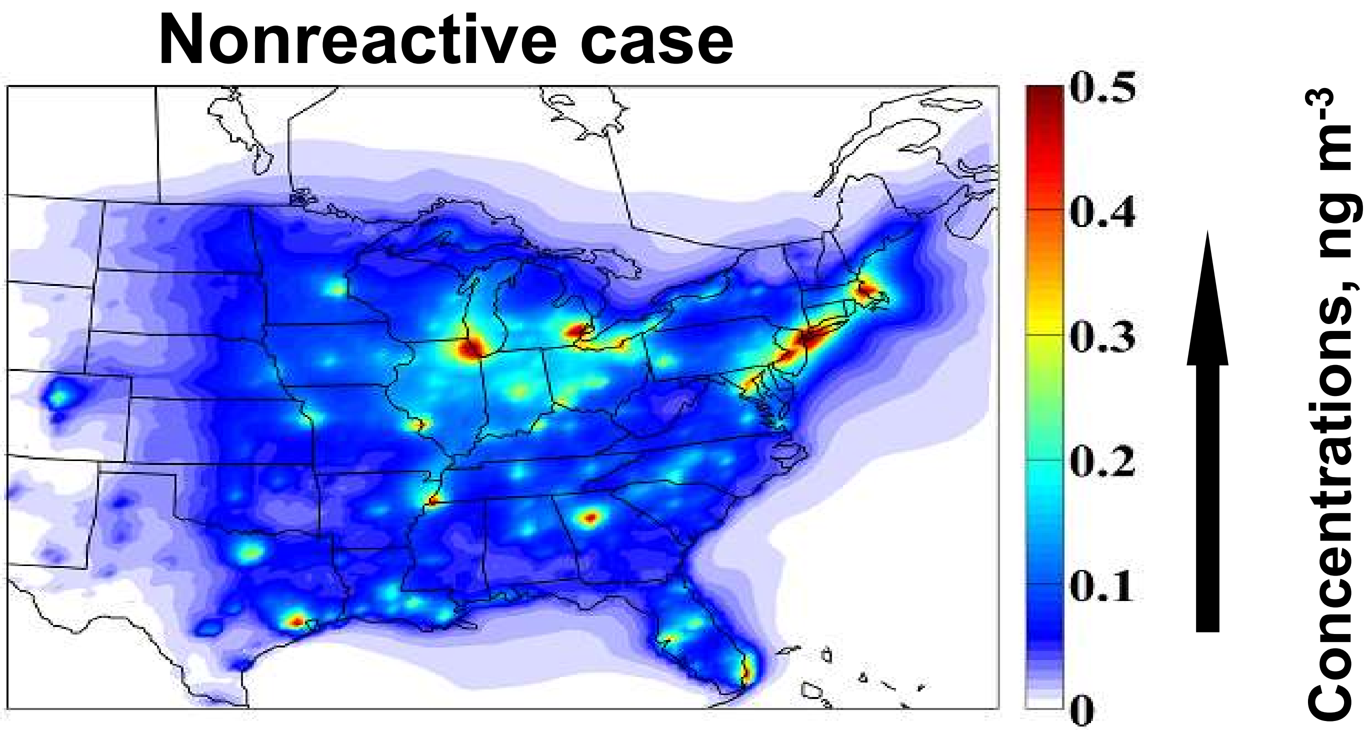
- Wide variability: norhopane oxidation is a heterogenous reaction phenomena depending upon gas-particle partitioning, OH update and particle size distribution

The PMCAMx modeling domain and episode



- Period of simulation : 12th to 28th July 2001
- Emissions: NEI'99 (EPA)
- Each grid cell 36 km x 36 km, 14 layers high up to 6 km

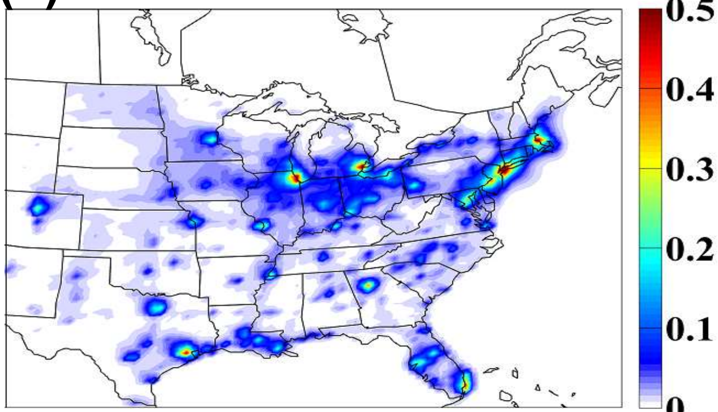
Norhopane concentrations



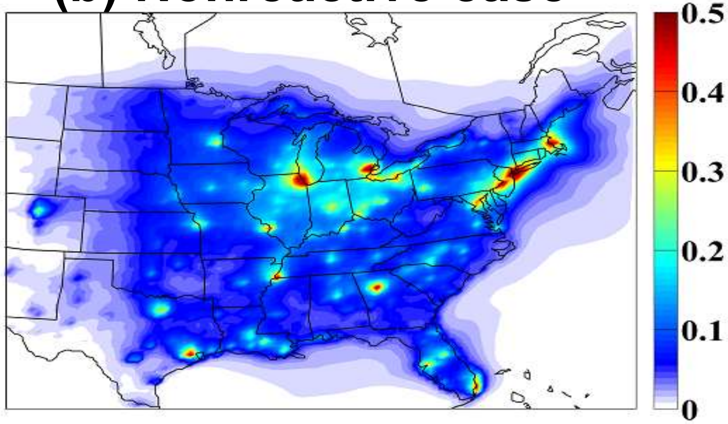
- Urban hotspots characteristic of high motor vehicle emissions

Effect of chemistry on regional norhopane levels

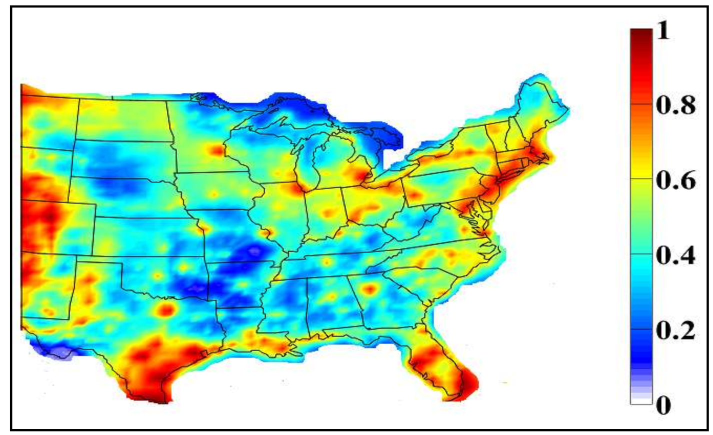
(a) Medium reactive case



(b) Nonreactive case

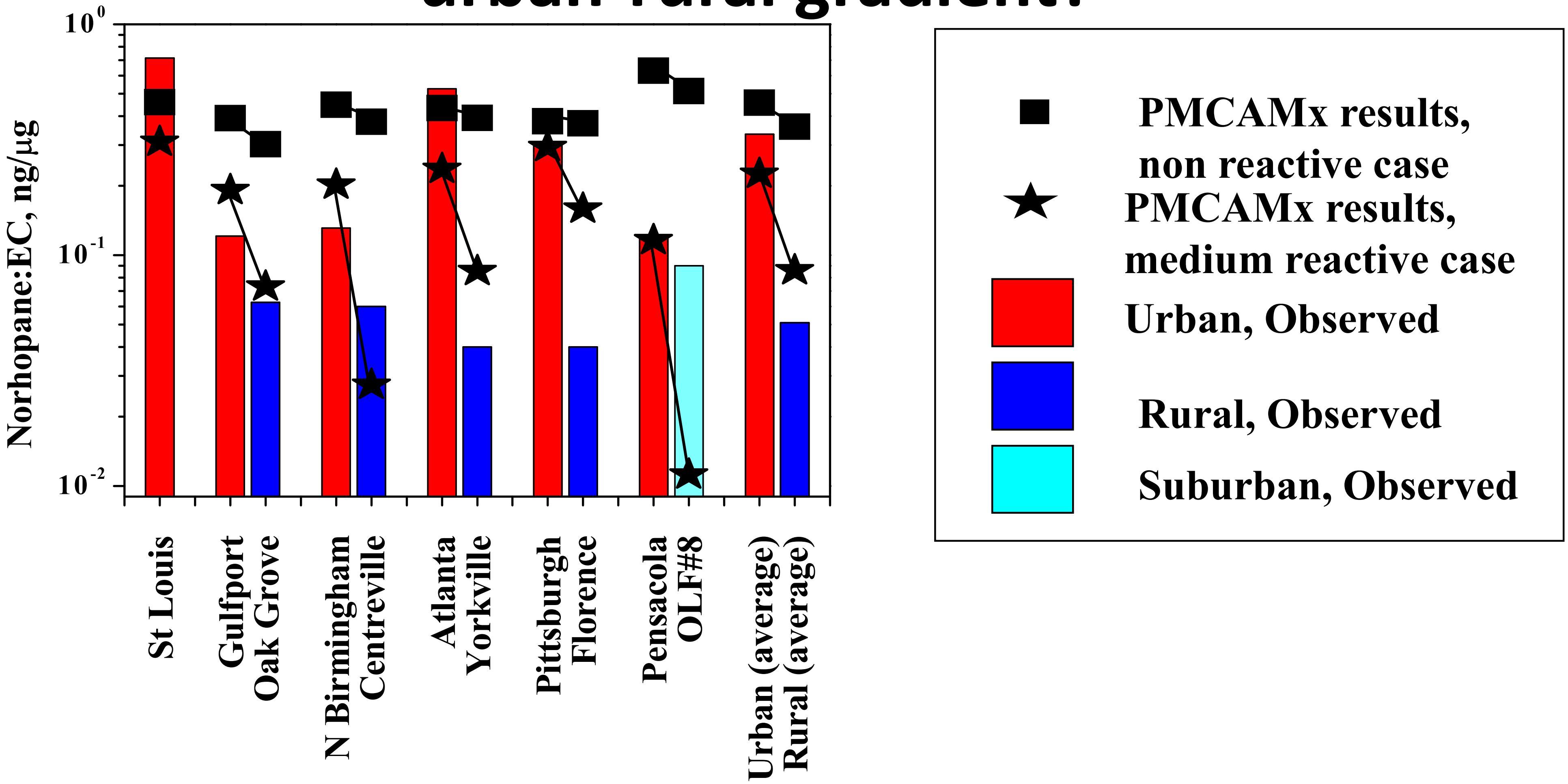


=



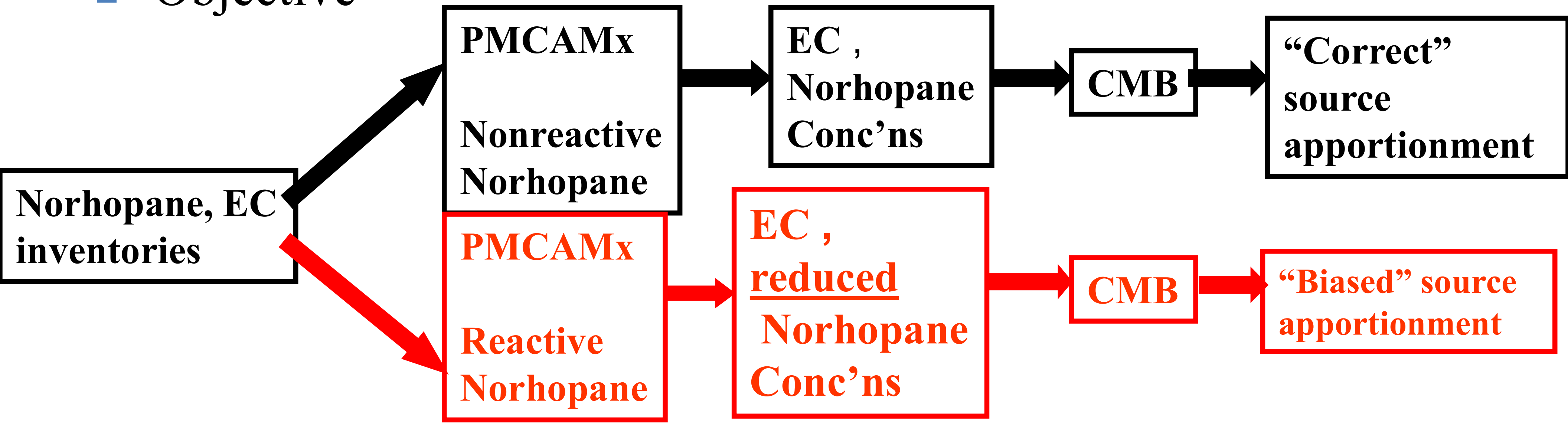
- **Fraction of nonreactive case : ~ 70% in the urban, 30% in the rural**
- **Transport increases time for photochemical processing during the urban-rural transit of an airmass resulting in lower concentrations**

How do the various scenarios reproduce the urban-rural gradient?

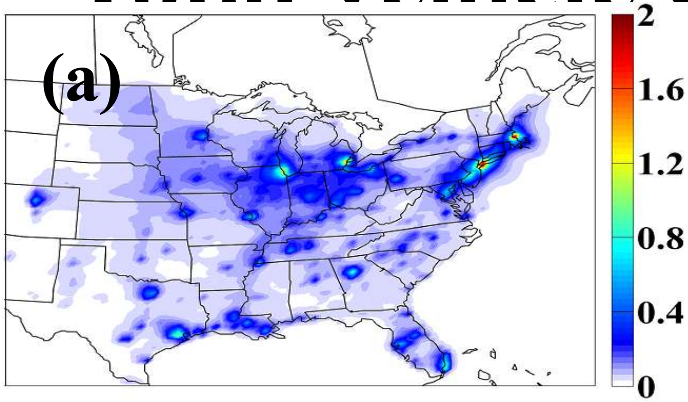


CMB analysis of PMCAMx data

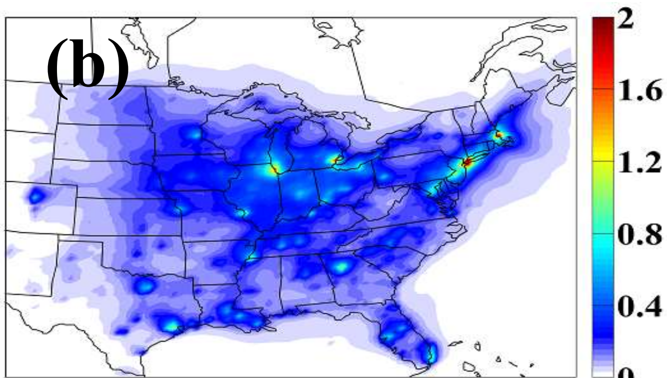
- PMCAMx output : synthetic ambient dataset for CMB
- Principle of CMB
- Balances for norhopane and EC
- Objective



Total vehicle OC : (Gas+Diesel)

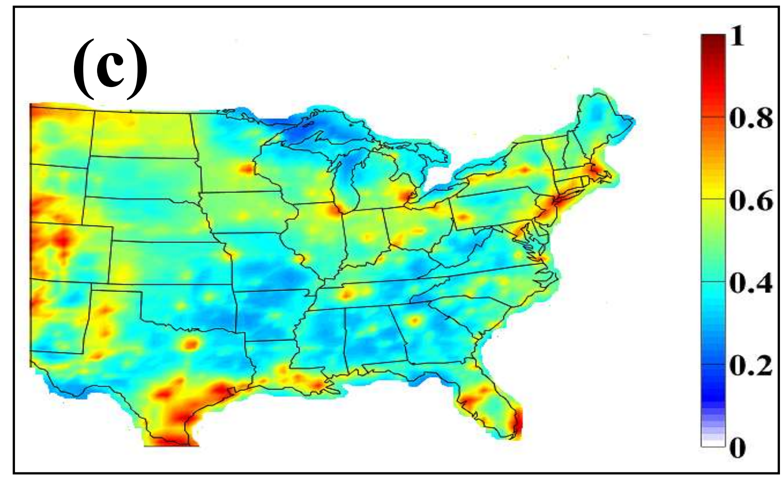


Total vehicle OC, medium reaction, µg m^{-3}, "biased"



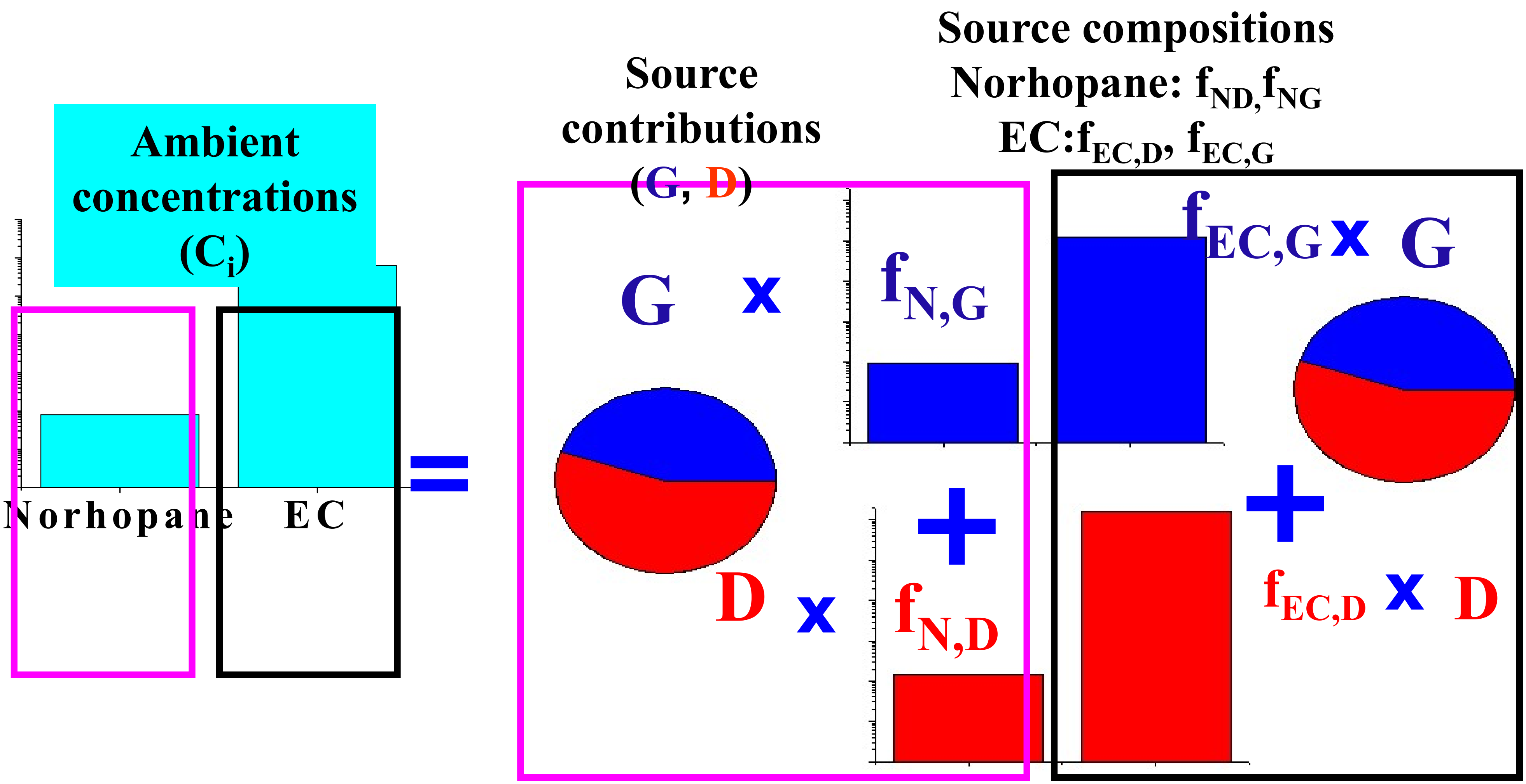
Total vehicle OC, no reaction, µg m^{-3} "correct"

=

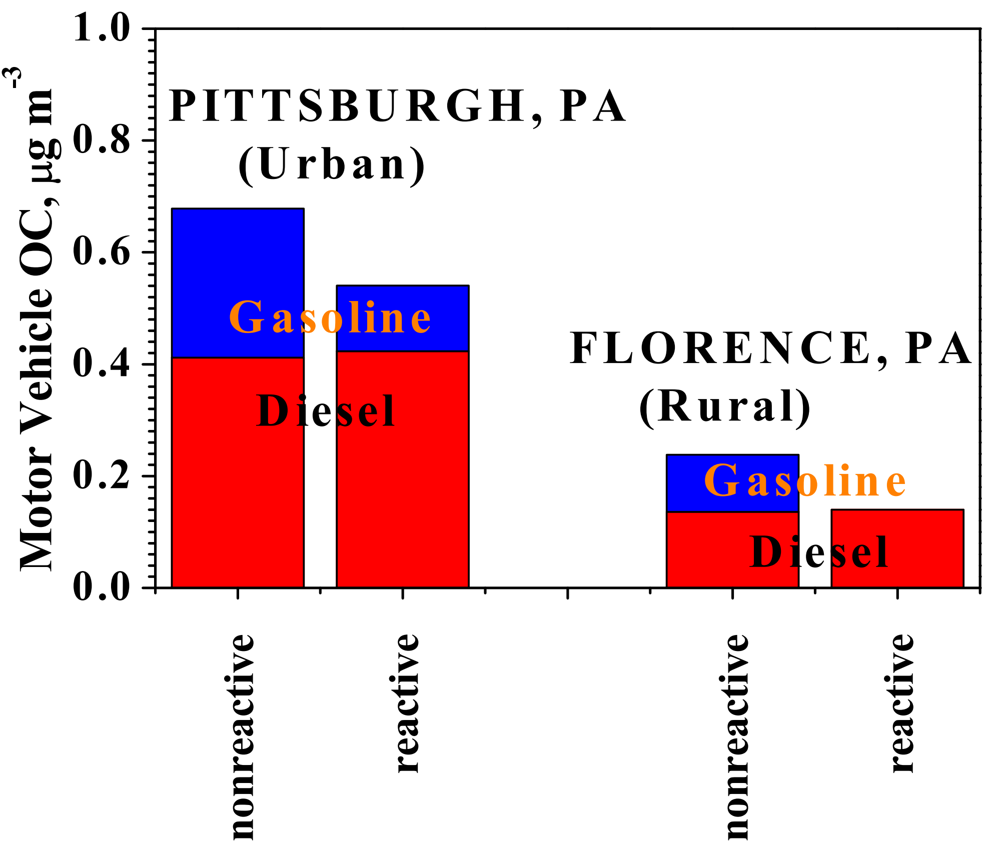


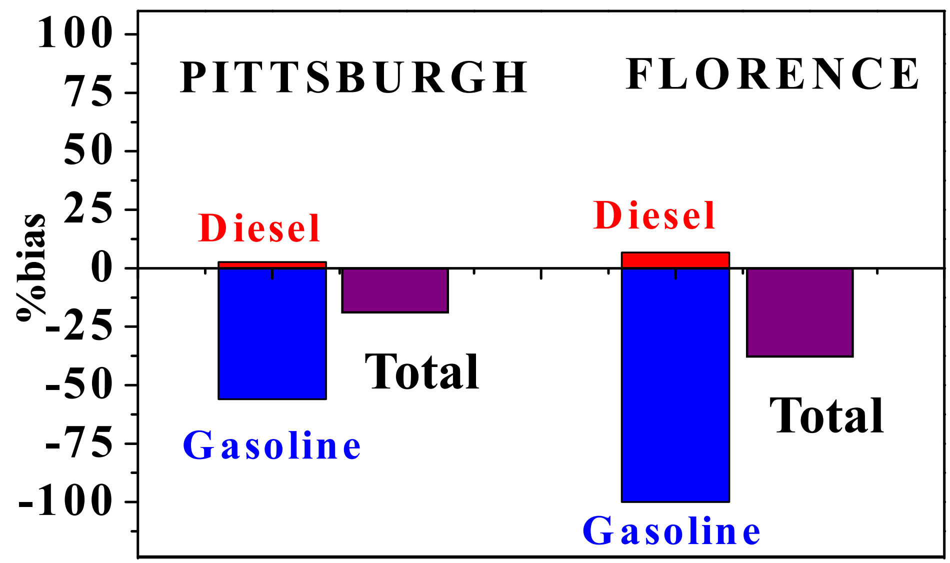
Ratio, (a)/(b)

Receptor Model : estimation of vehicular OC



What causes the bias in motor vehicle OC?





Reaction of norhopane →
i) underestimation of motor vehicle OC
ii) biases its gasoline-diesel split

Conclusions

- Modified a CTM to predict **summertime norhopane concentrations** in the Eastern US
- Reactive case : better job at urban-rural trend.
- Reaction : biases motor vehicle OC estimates:
  - Total vehicle OC, 20-40%, changes total OC by ~ 20%
  - Diesel, 1-10%, again not a big problem
  - **Gasoline : as high as 100%!!**
- Policy implications

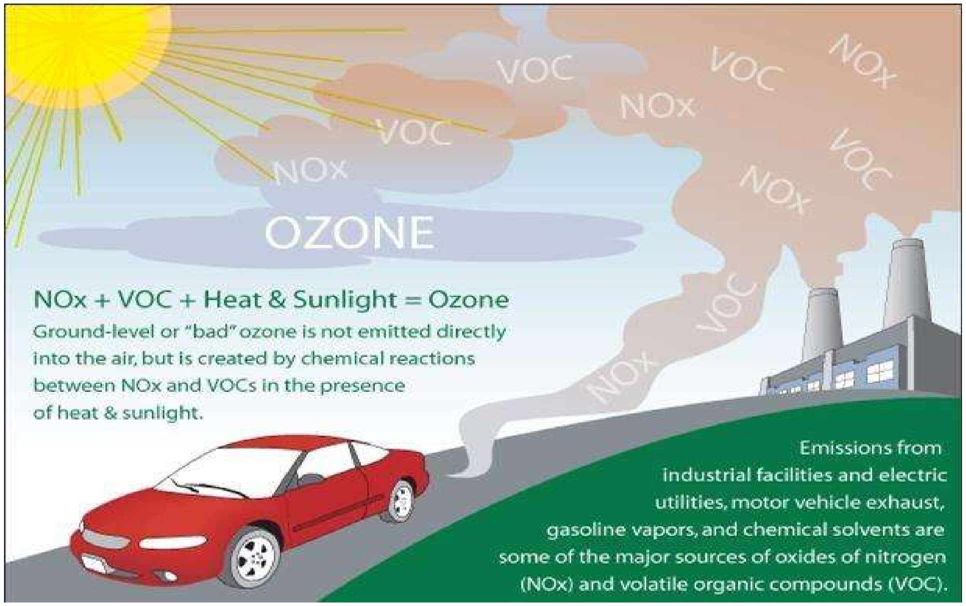
Policy Issues

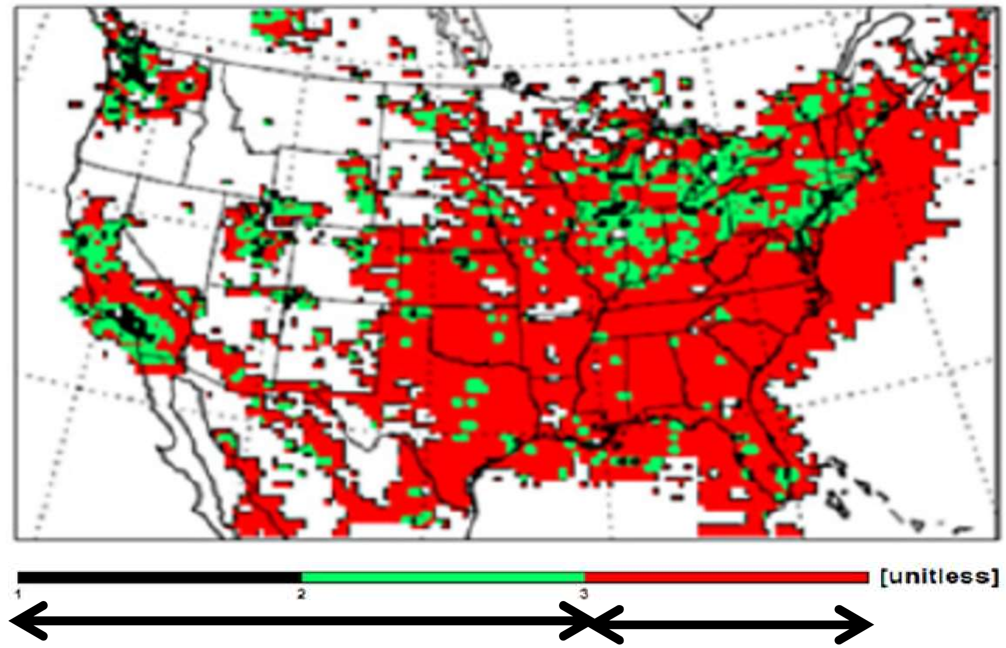
In the United States, efforts are mainly focused on trucks, buses, and larger diesel engines, which produce a major fraction of fine-particle emissions known as $PM_{2.5}$. Several Environmental Protection Agency (EPA) diesel regulations issued since 2000 will steeply reduce emissions by 2015. Besides requiring low-sulfur fuels, which reduce sulfates (a $PM_{2.5}$ component), the rules mandate that the heavy diesel fleet (including buses) be retrofitted with particle filters; EPA estimates costs at $400 to $1000 per vehicle. EPA expects that the majority of new diesel vehicles in 2007 will have particle filters. The devices generally work with a combination of a metal catalyst and a very hot multichannel trap in which soot particles burn off.

During the past 5 years, the U.S. diesel industry has put almost $5 billion into the development of better technologies. For example, researchers are working to find materials that are more resistant to the high temperatures needed to burn off the particles so the filters will last longer.

Kaiser, Science, 2005

Ground-level ozone



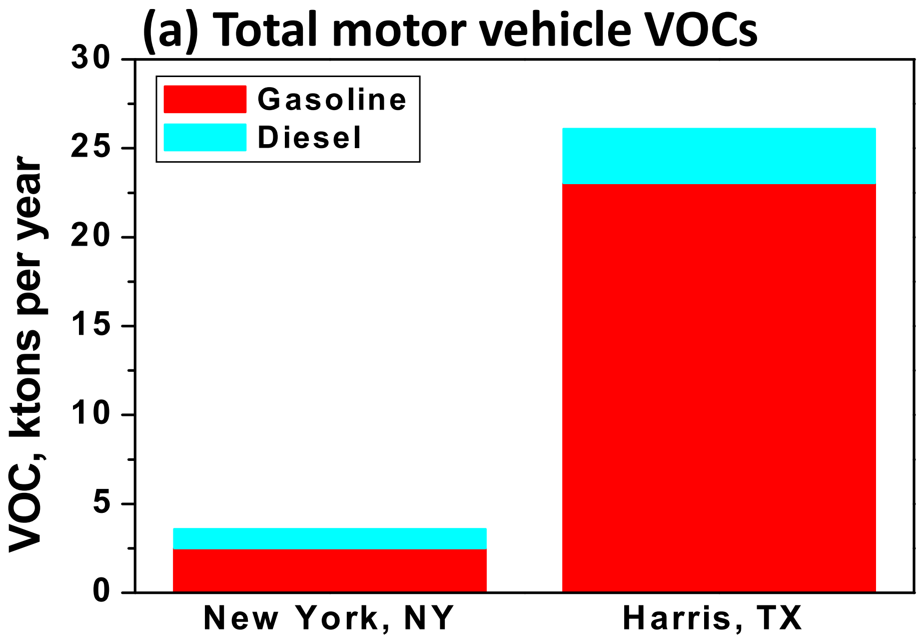


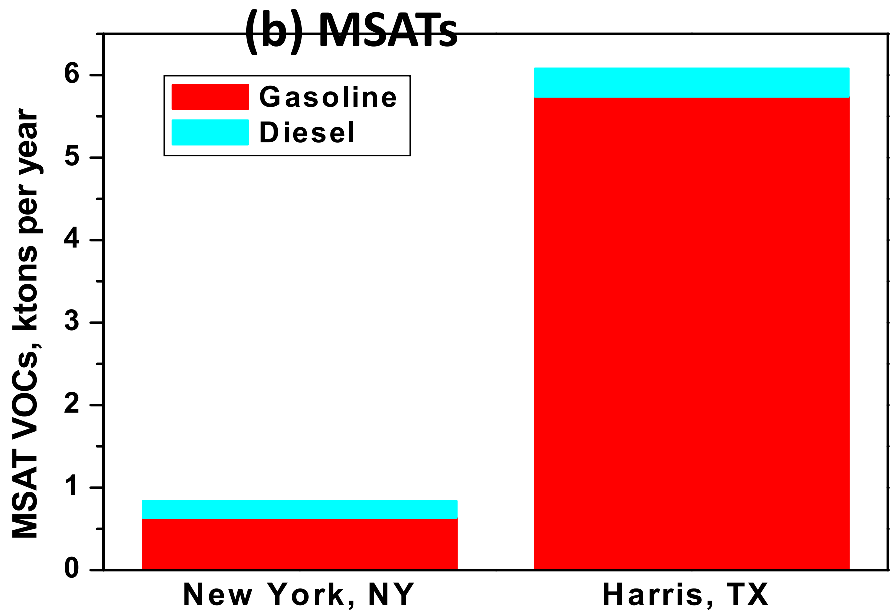
- VOC-sensitive: urban areas
- NOx-sensitive: rural areas, forests, petrochemical facilities

Choi et al., 2012

https://www.epa.gov/ground-level-ozone-pollution/ground-level-ozone-basics

Motor Vehicle VOC emissions

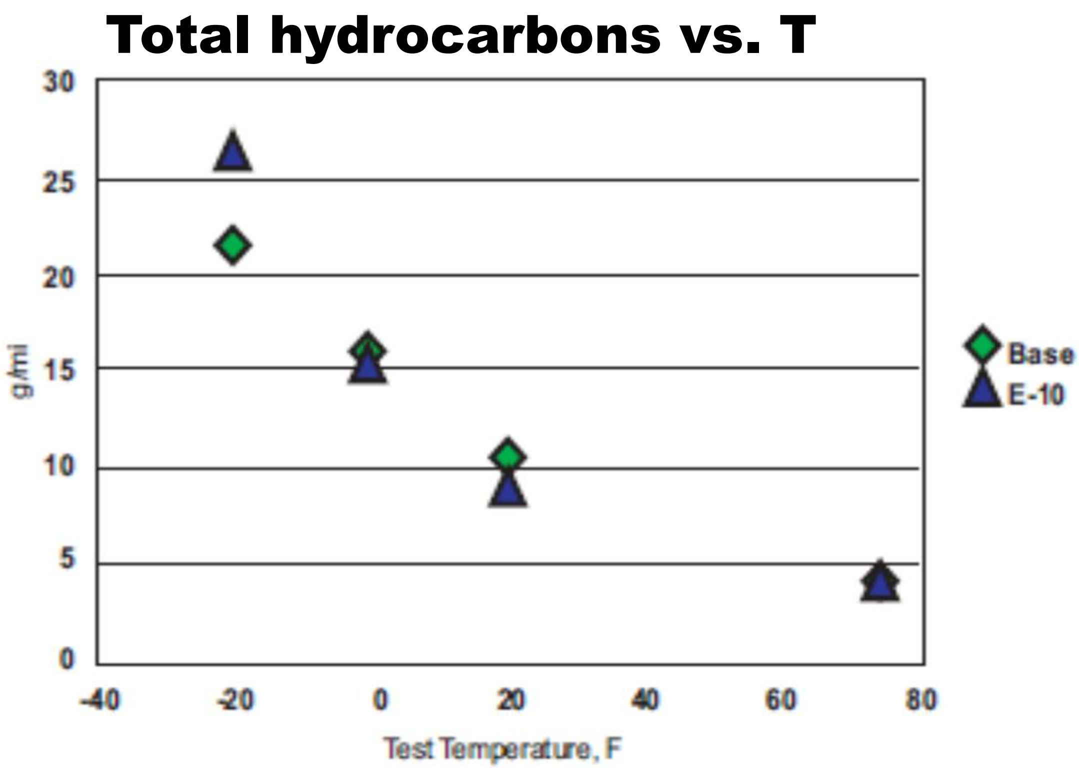




- Occupy around 25% of the total anthropogenic VOC share
- Two urban counties – New York (NYC-Manhattan) and Harris (Houston)
- Gasoline dominates the split for both VOCs and air toxics (carcinogenic species e.g. benzene, formaldehyde) emissions.

USEPA NEI, 2011

Temperature dependence of VOC emissions



Temperature ⬆ ⟶ Catalytic efficiency ⬆ ⟶ Emissions ⬇

Stump et al.

What is a speciation profile?

- Mass fractions of >100 VOC species emitted by a given source (e.g. gasoline exhaust).
- PM2.5 speciation relatively smaller: EC, OC, sulfate, nitrate.
- Imperative for air quality modeling: ozone and PM2.5 chemistry can differ widely among species.

Motivation for current work

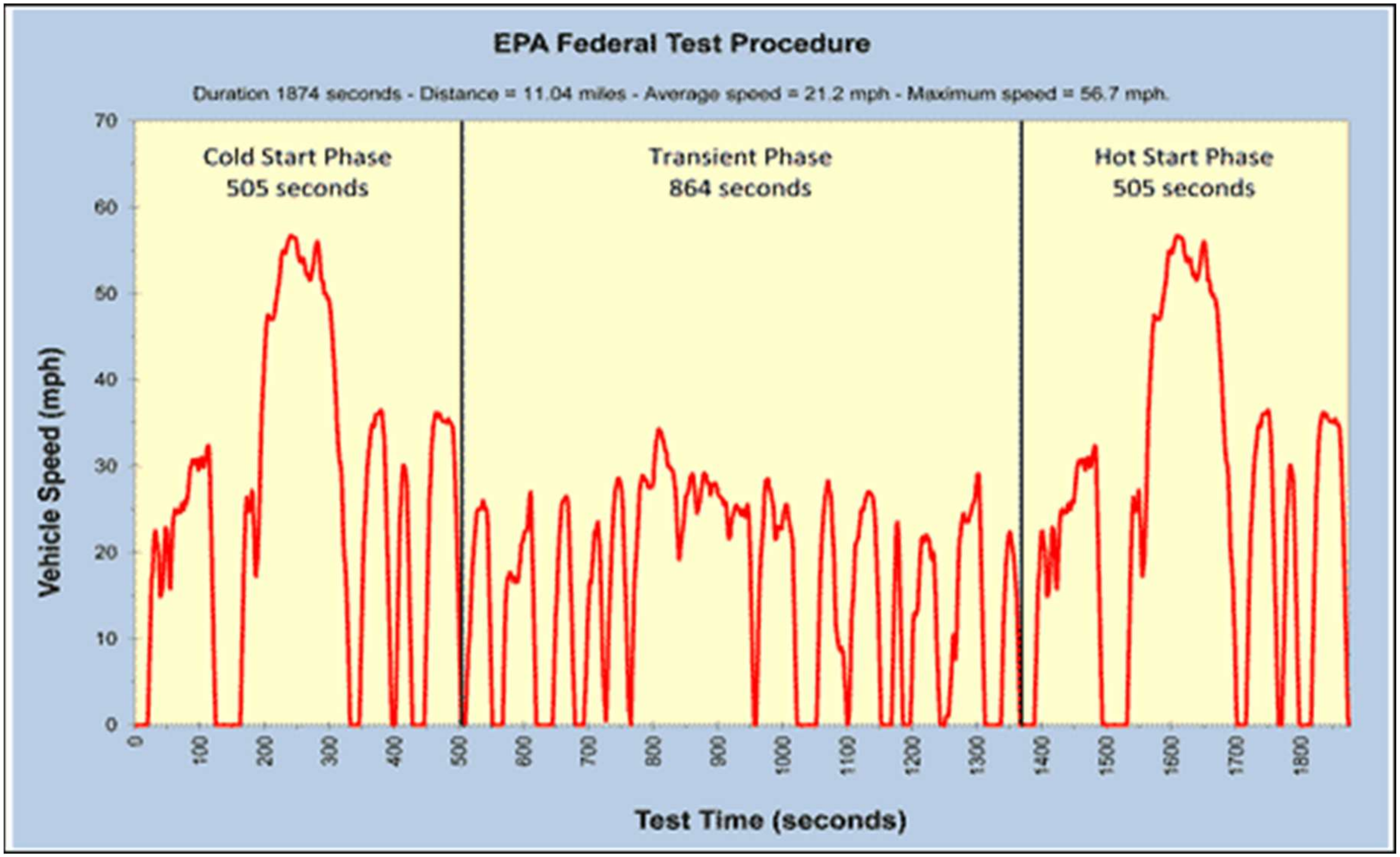
- Previous studies focused on temperature dependence of aggregate hydrocarbons and select MSATS .
- Little quantification of uncertainty in emission factors
- No comprehensive evaluation of speciation profiles - imperative for air quality modeling.
- This work intends to build on previous work to develop comprehensive temperature dependent speciation profiles.

Vehicle fleet

Name	Year	Technology	Standard	Mileage	Configuration
Buick Lucerne	2010	MPFI	Tier 2/Bin 4	22000	3.9L V-6
Jeep Patriot	2010	MPFI	Tier 2/Bin 5	22000	2.0L I-4
Kia Forte EX	2010	MPFI	Tier 2/Bin 5	25000	2.0L I-4
Mazda 6	2010	MPFI	Tier 2/Bin 5	24000	2.5L I-4
Mitsubishi Galant	2010	MPFI	Tier 2/Bin 5	38000	2.4L I-4

- Two driving cycles: FTP75 (urban driving) and US06 (aggressive driving)
- Three temperatures (0, 20 and 75^{o}F)
- Tested by URS on a chassis dynamometer at the Mercedes-Benz Research and Development North America Laboratory (Ann Arbor, MI) as part of an USEPA/OTAQ contract.
- Vehicles compliant with MSAT Cold Temperature Standard (NMHC EF: 300 mg mi^{-1} @20^{o}F).

Driving cycles: FTP75 for urban driving conditions



Driving cycles summary

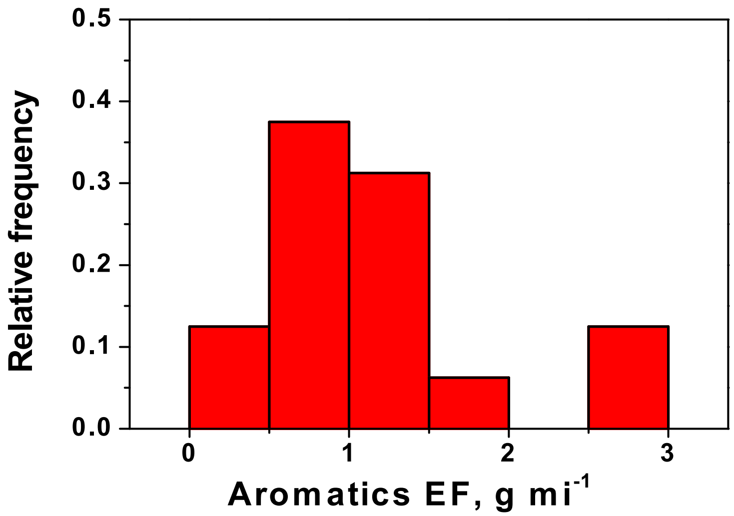
Quantity	Units	FTP75	US06
Sampling time	seconds	1874	596
Total distance	miles	7.45	8.01
Average speed	miles hour^{-1}	19.6	47.96
Maximum speed	miles hour^{-1}	56.7	80
Average Acceleration	ms^{-2}	0.5	0.67
Average Deceleration	ms^{-2}	-0.58	-0.73
% resting time	n/a	18.92	7.5
Stop frequency	# mi^{-1}	2.28	0.62

Argonne National Laboratory, 2008

Additional details

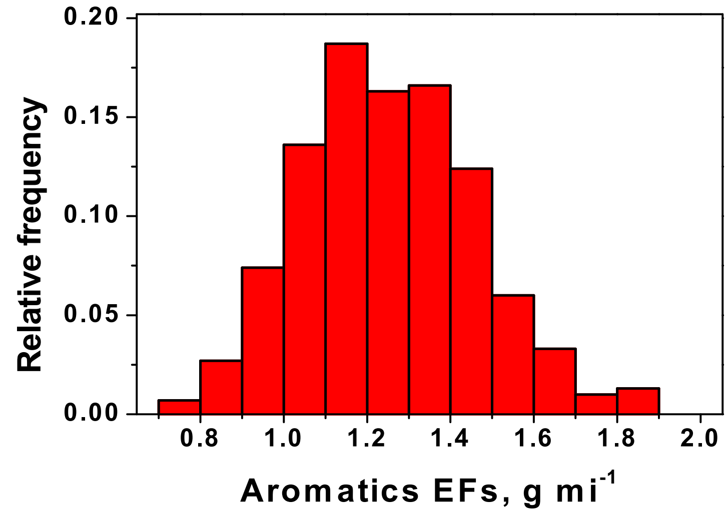
- Testing done at the USEPA's OTAQ premises.
- All vehicles used 10% ethanol by volume.
- 161 compounds, grouped into following species classes
  Aromatics
  Alkanes
  Cyclic Alkanes
  Alkenes
  Alkynes
  Ethers
  Aldehydes
  Ketones
- Methane evaluated separately
- FTP75 – 3 phases: Cold Start, Running and Hot Start.
- Cold Start evaluated separately

Bootstrap Method

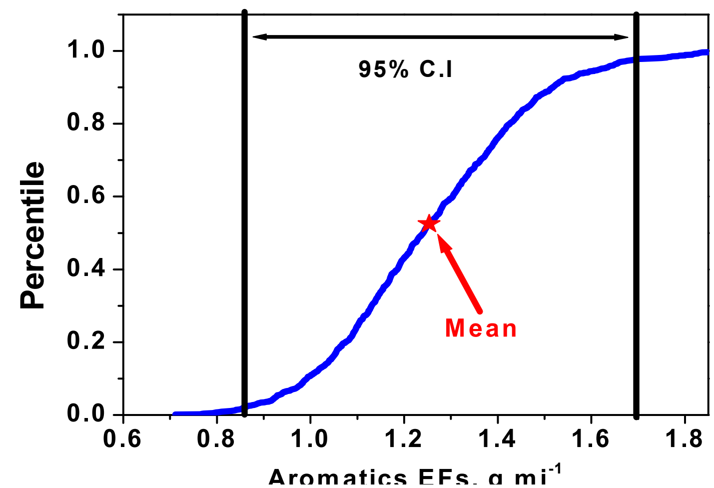


Draw Sample
Calculate Mean

Repeat 1000 times

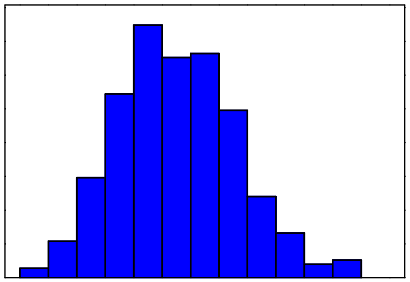


- Example with FTP Cold Start at 0°F.
- Distribution of means from random sampling.
- Uncertainty shown by 95% confidence interval.

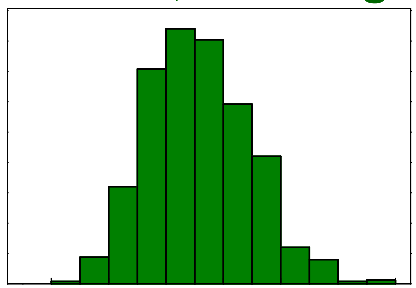


FTP Composite Emissions: Monte Carlo method

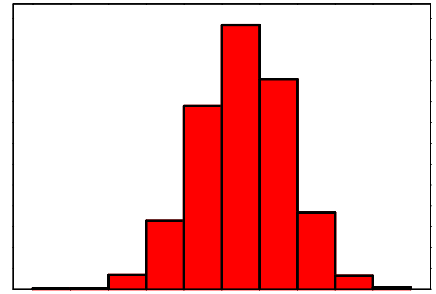
Means, Cold Start



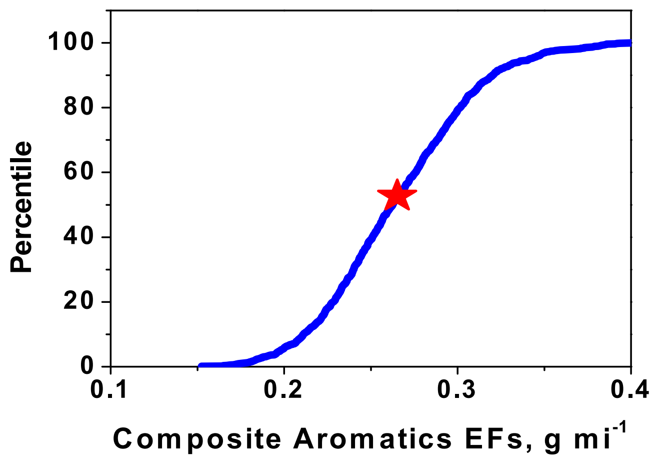
Means, Running



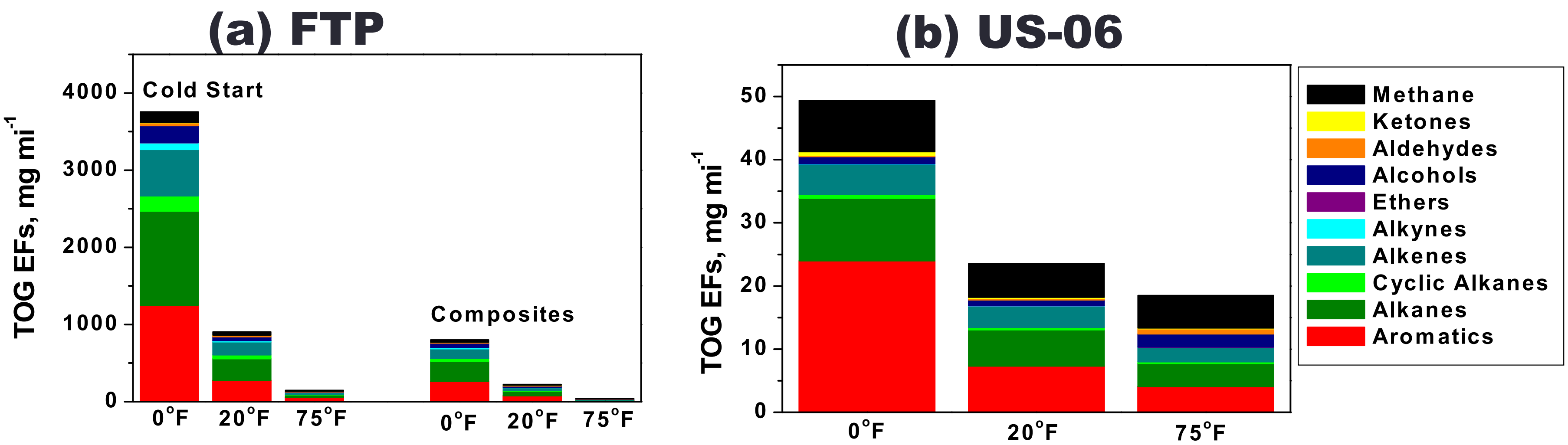
Means, Hot Start



0.43*Cold Start+Running+0.57*Hot Start



Temperature dependence of mean emission factors



- Significant decrease with temperature due to increasing catalyst efficiency.
- US-06 emissions significantly lower than FTP-Composite.

Uncertainty in mean emission factors

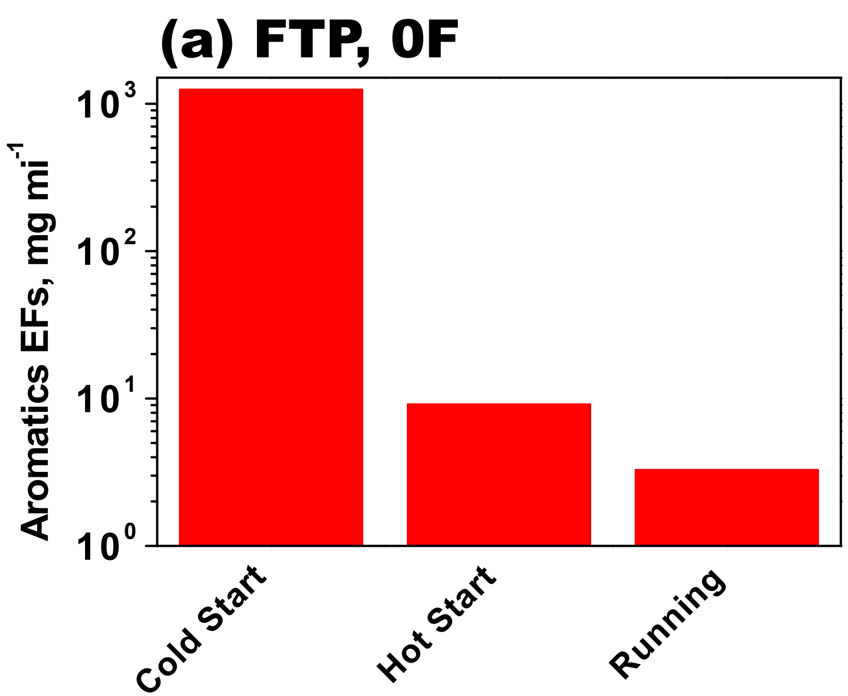
	0 ºF	20 ºF	75 ºF
Aromatics	265 (188-356)	51 (76-99)	12 (9-15)
Alkanes	256 (189-317)	61 (46-74)	8 (7-10)
Cyclic Alkanes	41 (25-59)	11 (7-14)	1.1 (0.8-1.3)
Alkenes	125 (100-150)	36 (26-46)	5 (4-6)
Alkynes	19 (14-24)	3.3 (2.3-4.3)	0.4 (0.2-0.6)
Alcohols	54 (39-69)	**18 (10-28)**	**7 (2-13)**
Aldehydes	9 (8-11)	7 (6-8)	3 (4-11)
Ketones	1.2 (1-1.3)	1.7 (1-2.5)	0.6 (0.5-0.7)
Methane	34 (29-39)	12 (9-14)	5 (3-7)

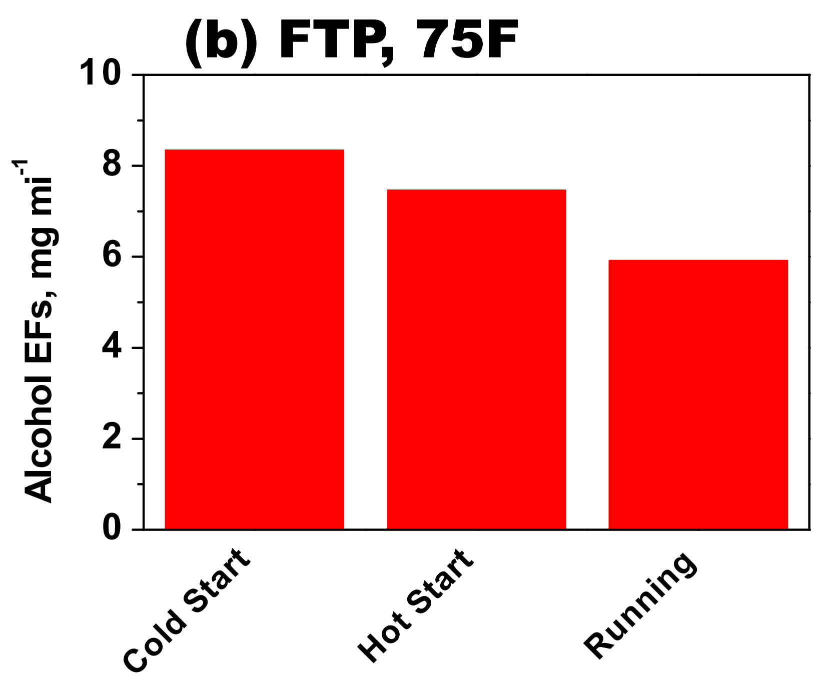
- Uncertainty quantified by endpoints of 95% confidence interval: 2.5th and 97.5th percentiles
- Example with FTP75 composite emissions, units in mg mi^{-1}.
- Broadly factor of 2, uncertainty.

What influences composite emissions?

- **Two scenarios:**
- **CASE 1 :** Cold Start dominates by orders of magnitude.
- ***Applicable to most hydrocarbons at all temperatures*.**

- **CASE 2:** Hot Start and Running comparable to Cold Start.
- ***Applicable to all oxygenates - alcohols, aldehydes and ketones.***

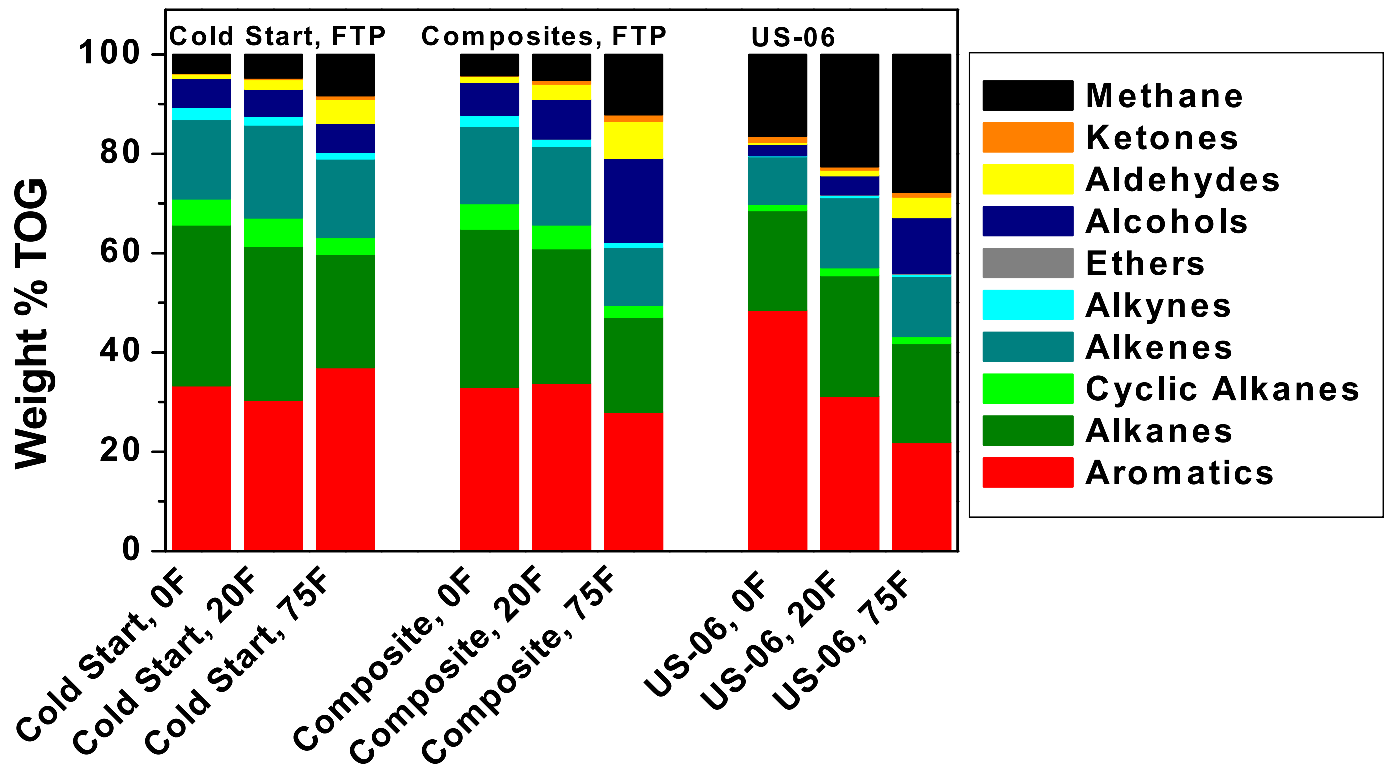




Conclusions

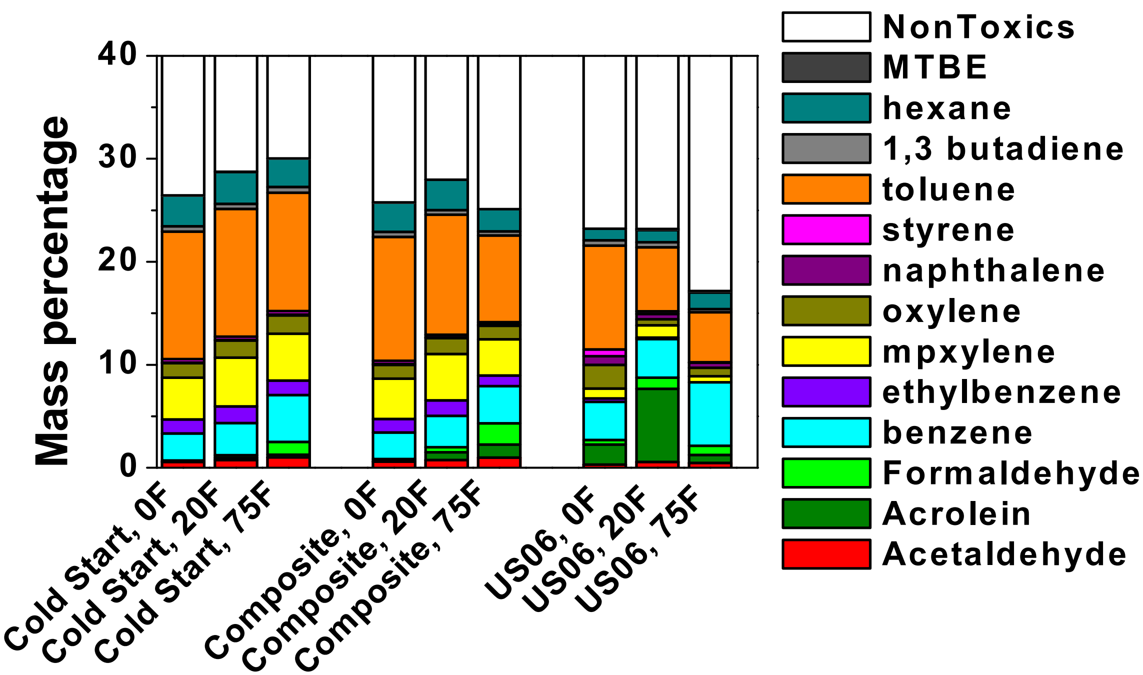
- Significant difference in speciation across temperatures and driving conditions.
- Cold Start emissions were the dominant FTP phase for most hydrocarbons, greater by at least 2 orders of magnitude than Running and Hot Start emissions .
- For alcohols and carbonyls, Cold Start, Running and Hot Start emissions were comparable.
- Toxics speciation: benzene and oxygenates fraction rises, toluene fraction falls with temperature.

Speciation profiles



- Significant increases seen in speciation for alcohols, aldehydes and methane.
- Alkanes show definitive decrease with temperature for both Cold Start and composite phases of the FTP cycle.
- Aromatics significantly fall with temperature for the US-06 cycle.

Speciation profiles and patterns



- Broadly, benzene and oxygenates fractions rise, toluene fraction falls with temperature.
- **Cold Start:** toxics fraction rises marginally with temperature, from 26% at 0°F to 30% at 75°F.
- **FTP75 Composite:** Changes within margin of error.
- **US06:** Toxics fraction drops significantly from 23% at 0°F to 17% at 75°F, due to fall in toluene fraction.

Marcellus shale natural gas

- Significant energy deficit in the US – heavy research focused on exploring candidate energy technologies
- Shale – impervious rock encases significant amount of natural gas
- Needs to be hydraulically fractured or "fracked" to release the gas, typically done by frac pumps (10-15 locomotive engine sized equipment, 1000-2000 hp), using fracturing fluid (complex mixture)
- Largest reserves in the Marcellus Shale region

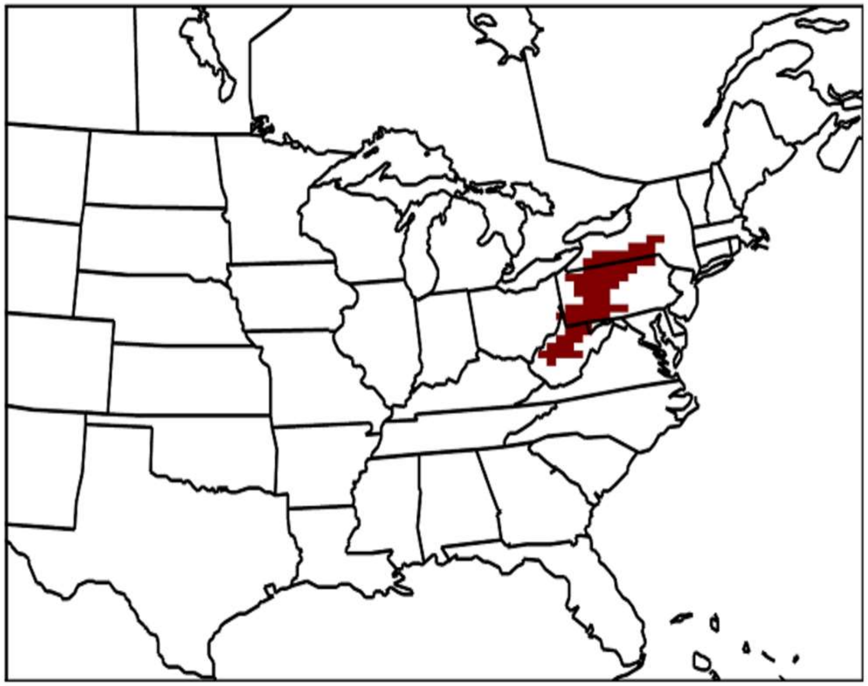
Natural gas development: typical emission sources

Well development

Gas production

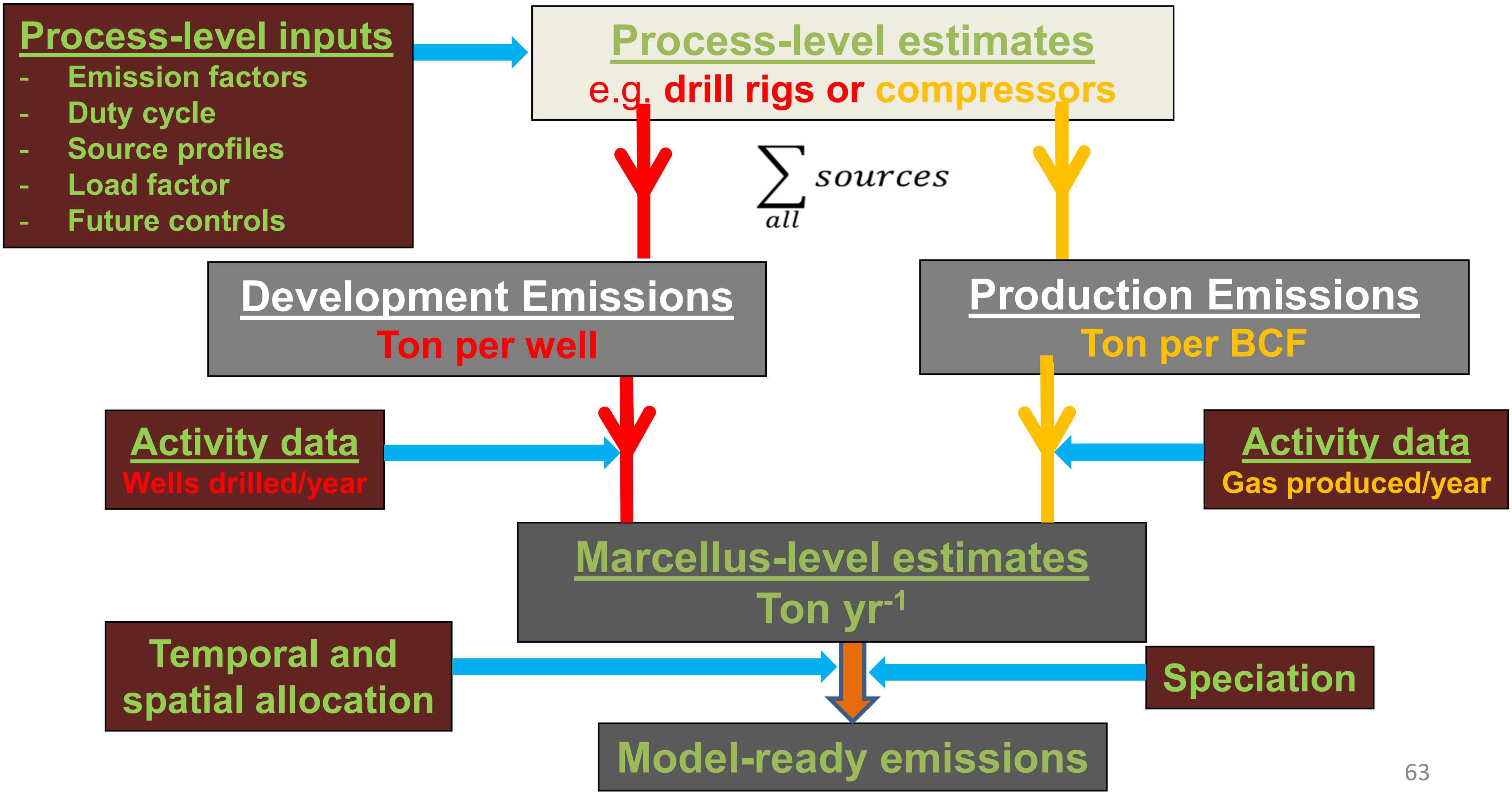
Midstream

Simulation domain and Marcellus region



- Not included MD and OH due to lack of projection data

Multi-tiered approach



Data sources

Direct data

- E.g. Emission factors for trucks

Surrogate emission factors

- Heavy duty diesel engines like locomotives and generators: surrogates for drill rigs and frac pumps

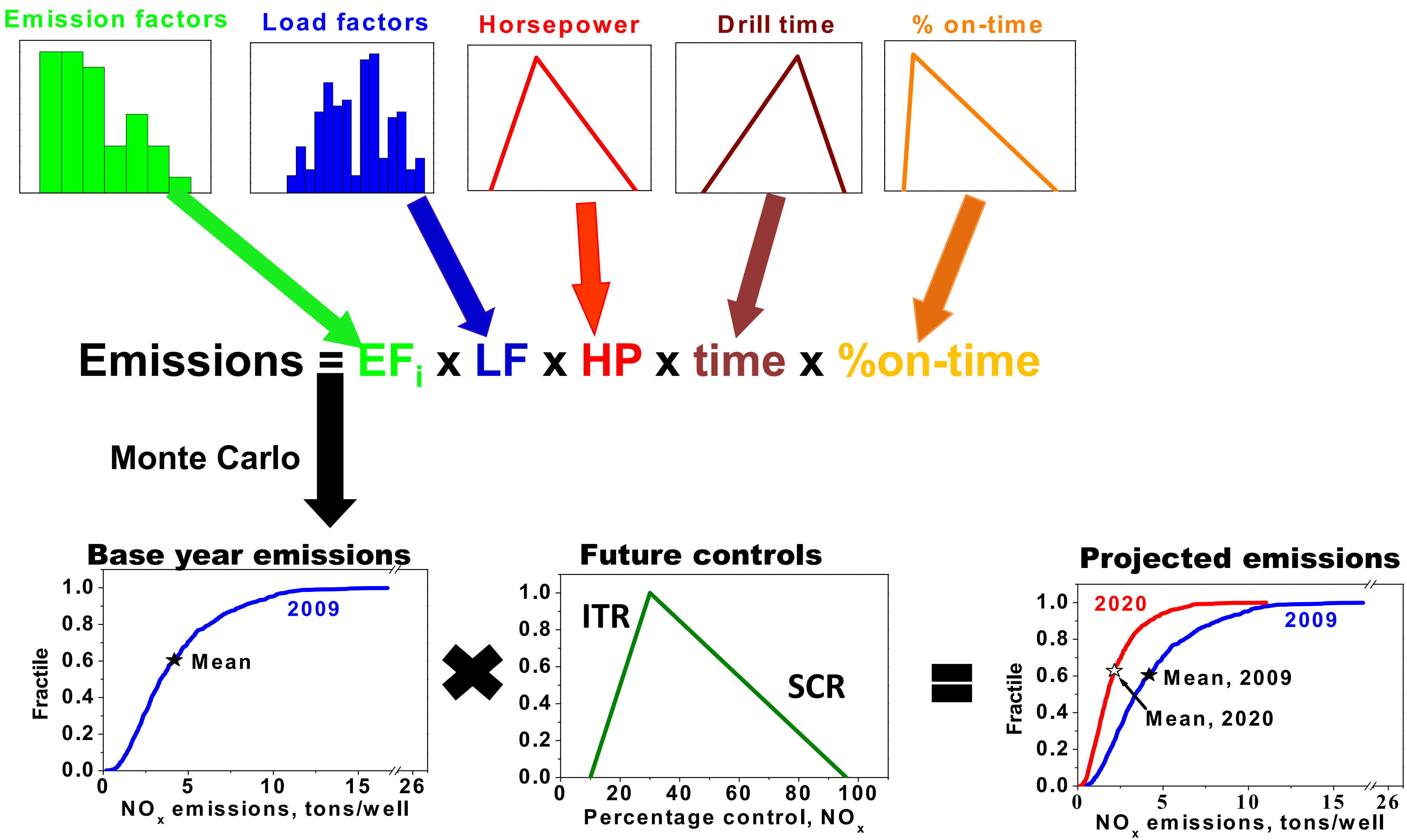
Activity data

- PADEP, WVGES, NYDEC, some companies (e.g. Chesapeake Energy Corporation, EQT)
- Well drilling and gas production forecasts (Considine et al., 2009, 2011; Considine, 2010; NETL, 2010; EIA, 2012)

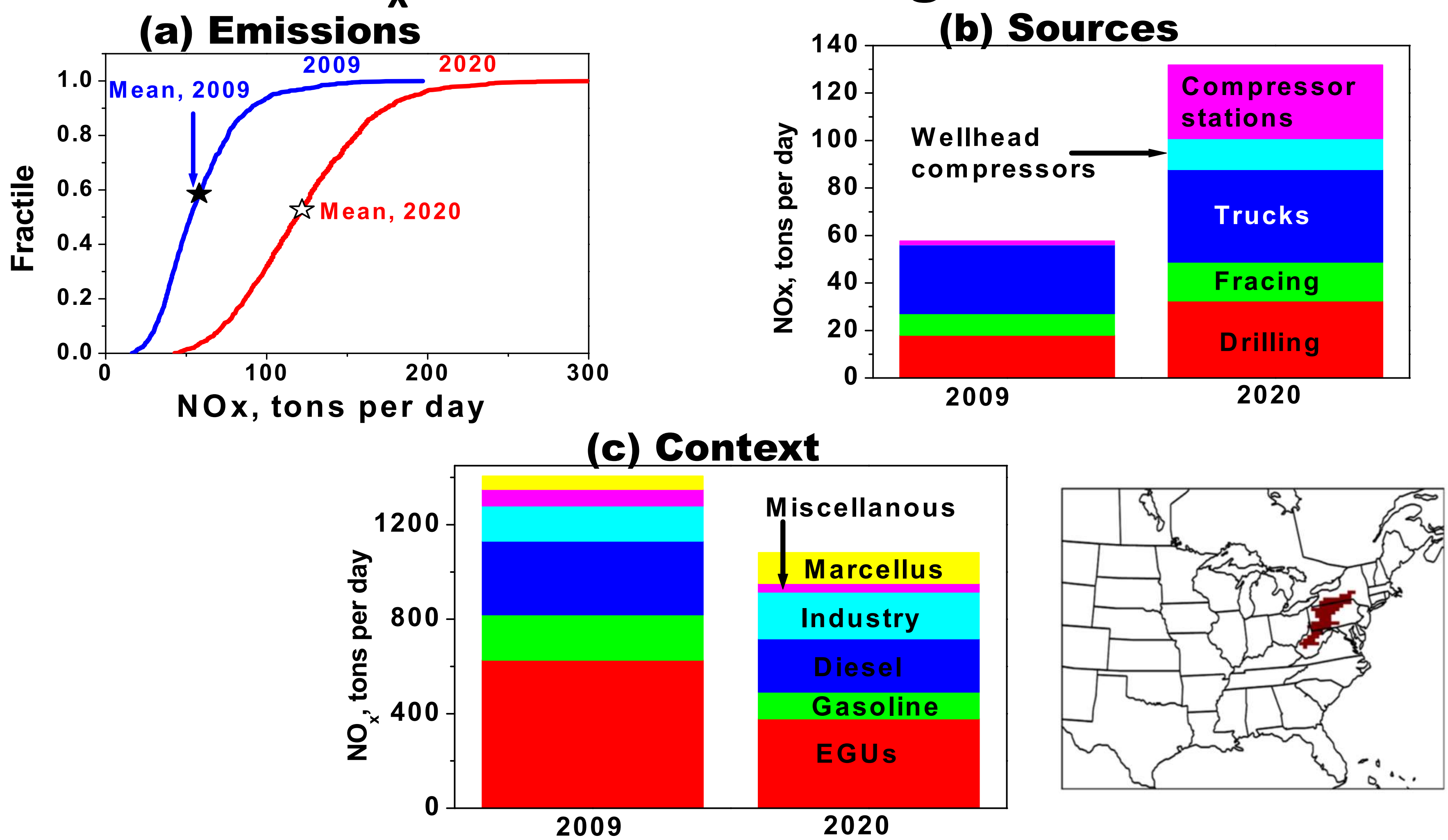
Other natural gas inventories

- Haynesville Shale (Grant et al., 2009)
- CENRAP inventory (Bar-Ilan et al., 2008)
- State of TX (Baker & Pring, 2009)

Schematic for NOx emissions per unit well



NO_x emissions and regional context



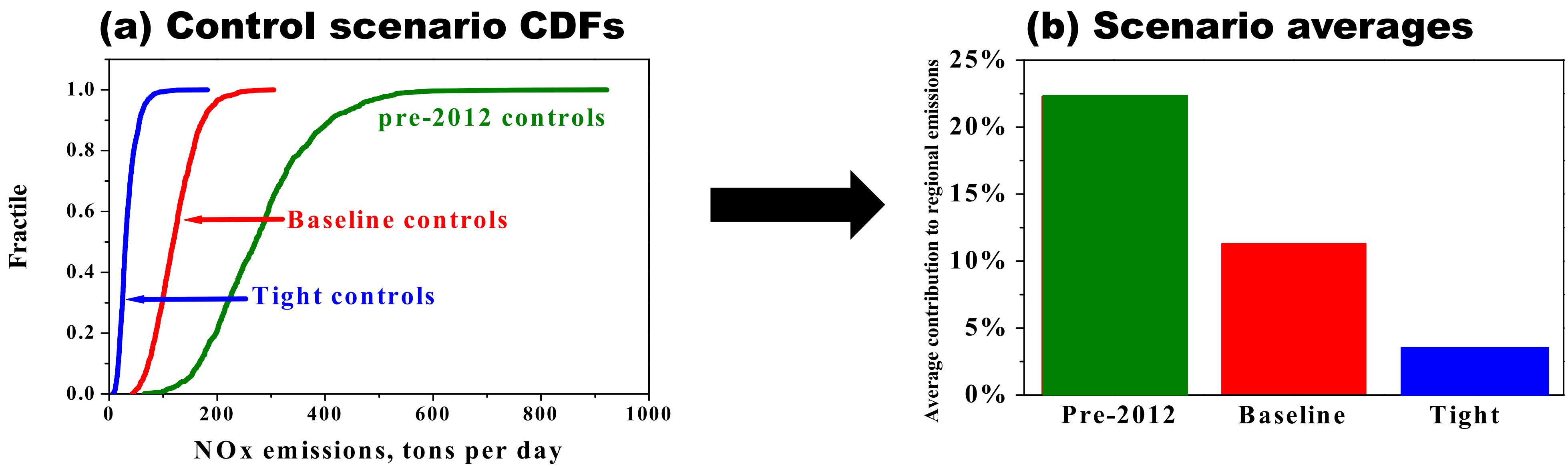
Control scenarios

- **Pre-2012 controls** scenario uses control technologies pre-dating regulations before 1st of January, 2012
- **Baseline controls** scenario assumes that the equipment fleet has a distribution of controls
- **Tight controls** scenario assumes that all equipment uses control technologies which result in the highest reduction in emissions

Effects of Emission Control technologies and regulations

- Selective Catalytic Reduction (SCR) for NOx emissions from drilling, fracing, trucks and compressors, 95% reduction
- Vapour Recovery Units for condensate tanks and green completion for wells, more than 97% VOC capture.
- Regulations- Tier 4 (~ BS6) for nonroad equipment, Oil and Gas Rule for oil and natural gas development. Both come into effect in 2012.

Effects of controls on NOx emissions

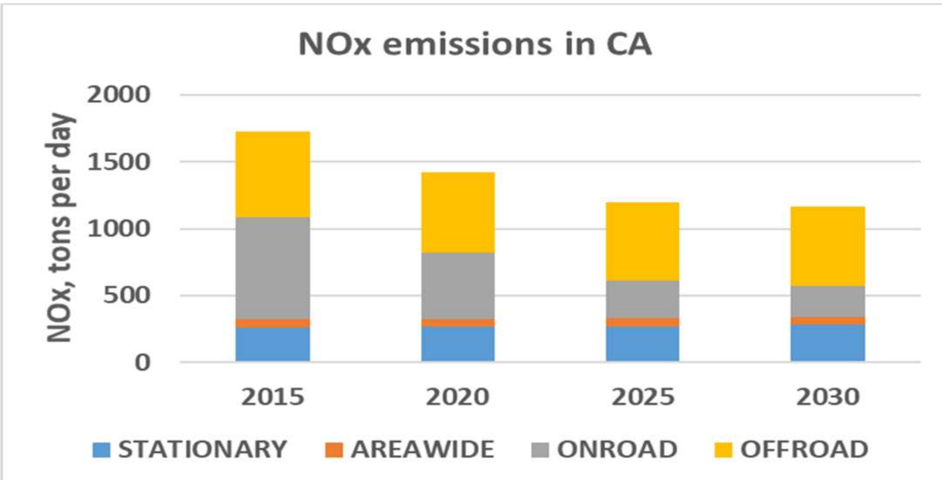


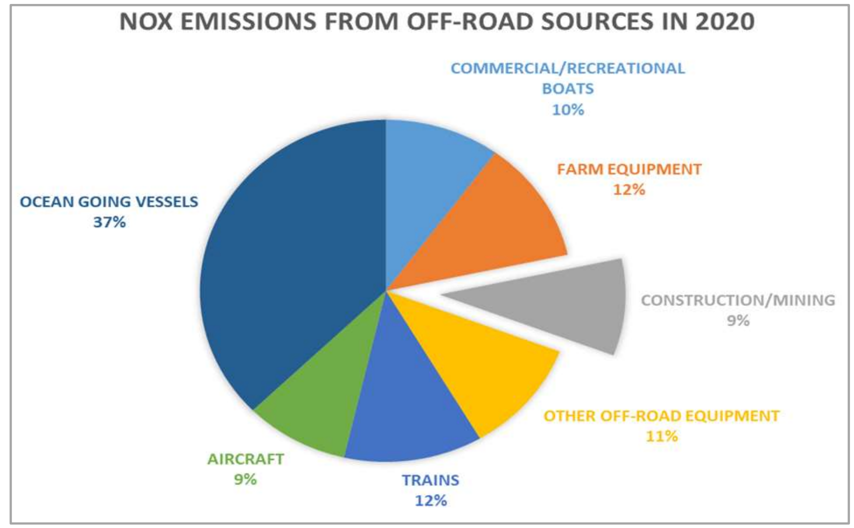
- Similar percentage contributions observed for VOCs and EC

Conclusions

- Constructed an emissions inventory for natural gas development in the Marcellus Shale for criteria pollutants.
- Development could contribute 11% of regional NOx emissions, equaling emissions from gasoline vehicles.
- Elemental carbon emissions due to Marcellus development could significantly offset projected reductions due to controls.
- Uncontrolled emissions could prove to be a major contributor to regional NOx, VOCs and EC emissions (all around 25 % of regional).
- Stricter control technologies could significantly reduce this impact (less than 5%).

Projected NOx emissions in California





- Slower decrease in off-road emissions than on-road
- Off-road sector is projected to occupy ~40% of the emission mix in 2020
- Construction equipment contribute to 9 % of the off-road NOx inventory

https://www.arb.ca.gov/orion/

Equipment specific emissions and load factor

$$E_{Species,i} = EF_{Species,i} \times P_{Rated} \times LF_i \times A_i$$

Species source emissions, tons per day

Species emission factor, g hp^{-1}hr^{-1}

Rated Power

Load factor

Activity, hrs/day

$$LF\,(true) = \frac{P}{P_{Rated}}$$

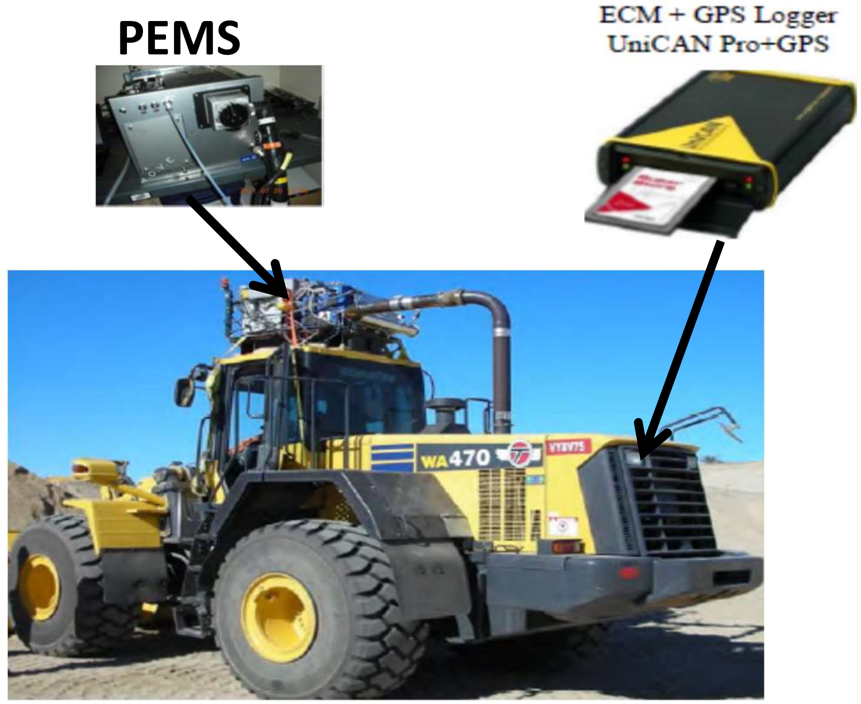
Definition

$$LF\,(surrogate) = \frac{S - S_{min}}{S_{max} - S_{min}}$$

Surrogate methods:

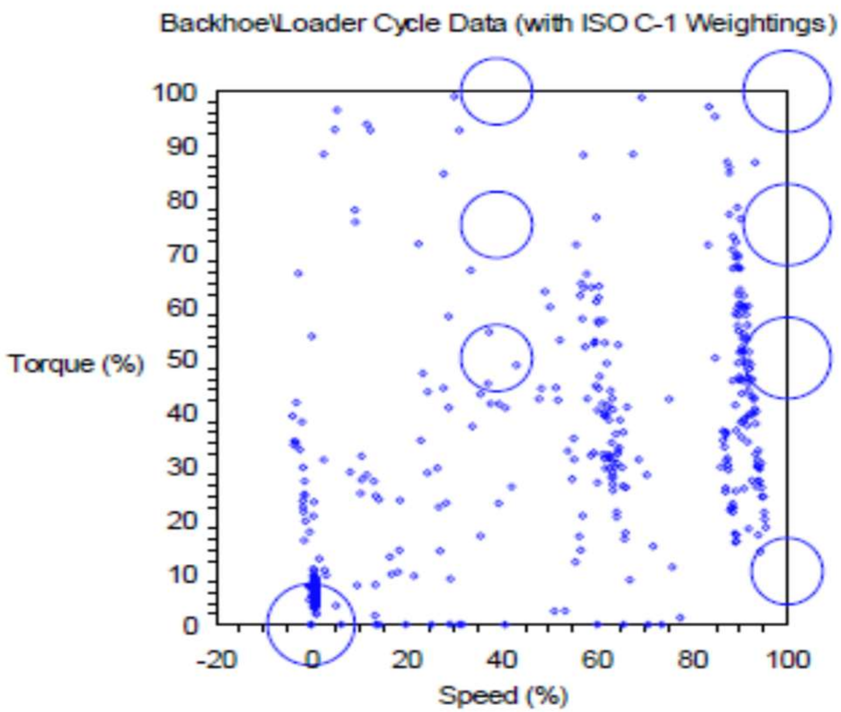
- Used in absence of load information
- Typical surrogates:
  - Engine speed
  - Throttle valve position
  - Fuel consumption

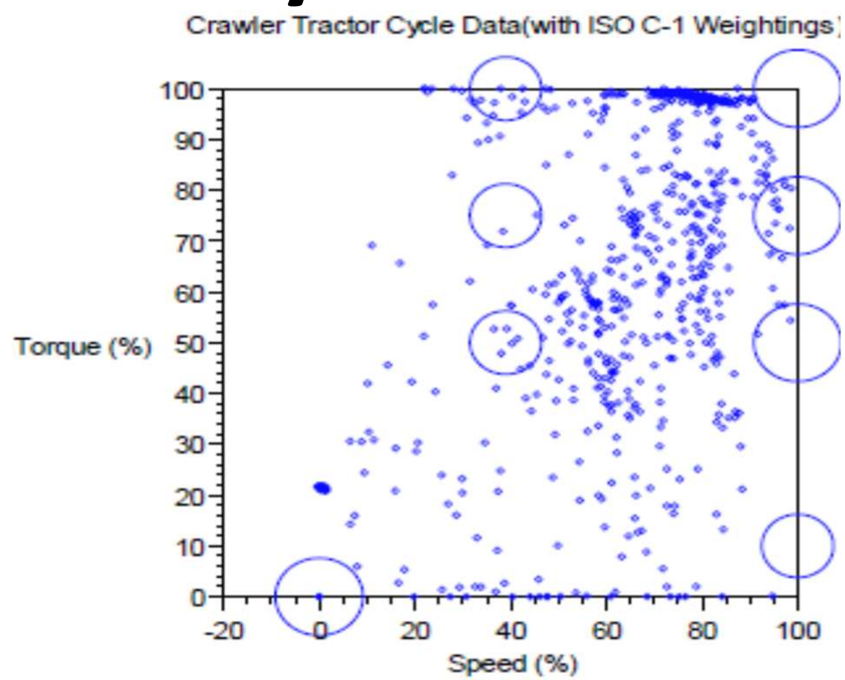
In-use data collection protocol



- Portable Emissions Measurement Systems (PEMS): CO2, NO_x, $PM_{2.5}$, THCs, CO
- DataLogger : 150+ parameters. E.g. lat-lon, velocity, fuel rate, **engine load**.
- Data collected at 1 Hz frequency

Real-world activity data vis-à-vis standard certification cycles

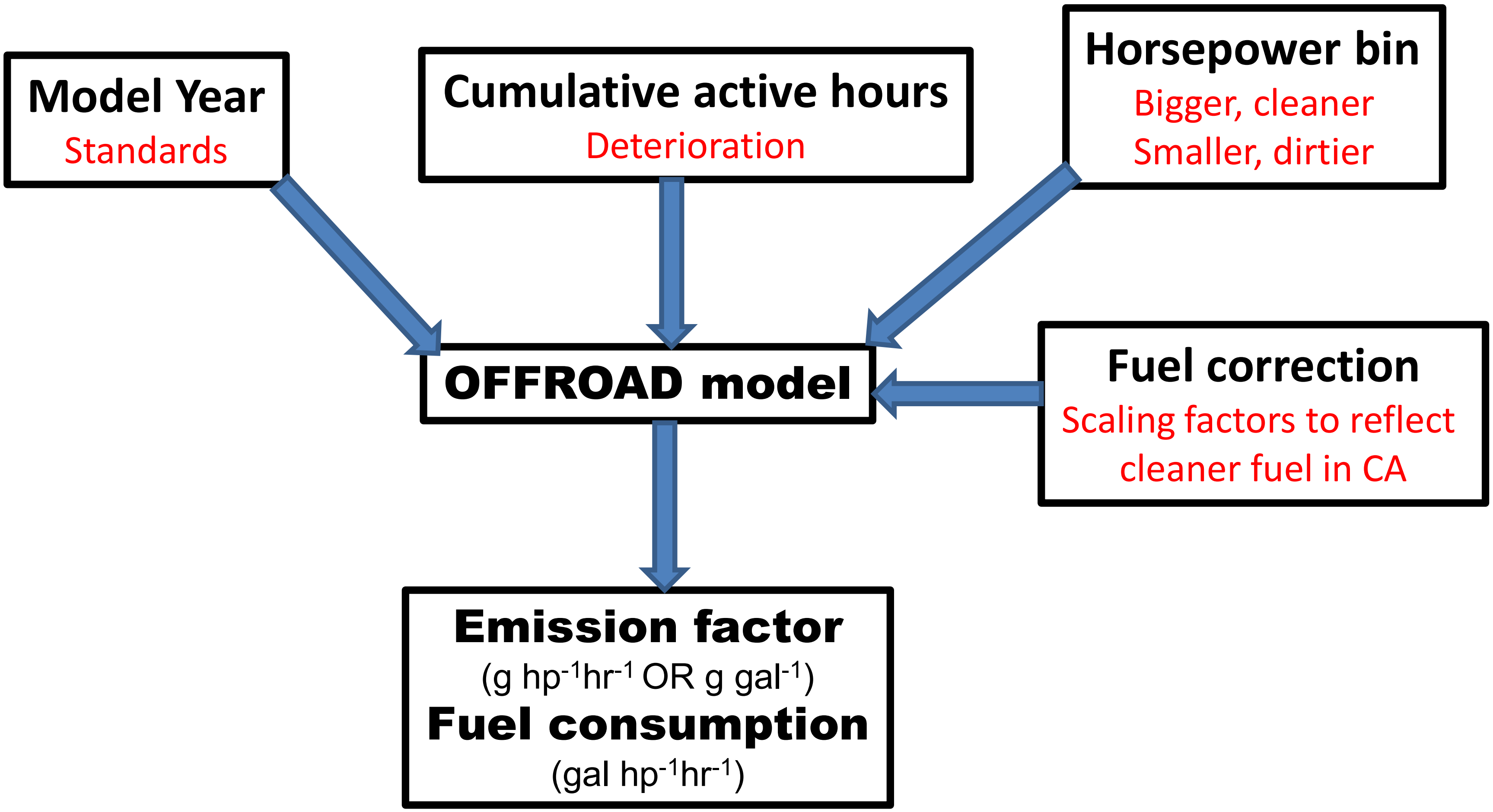




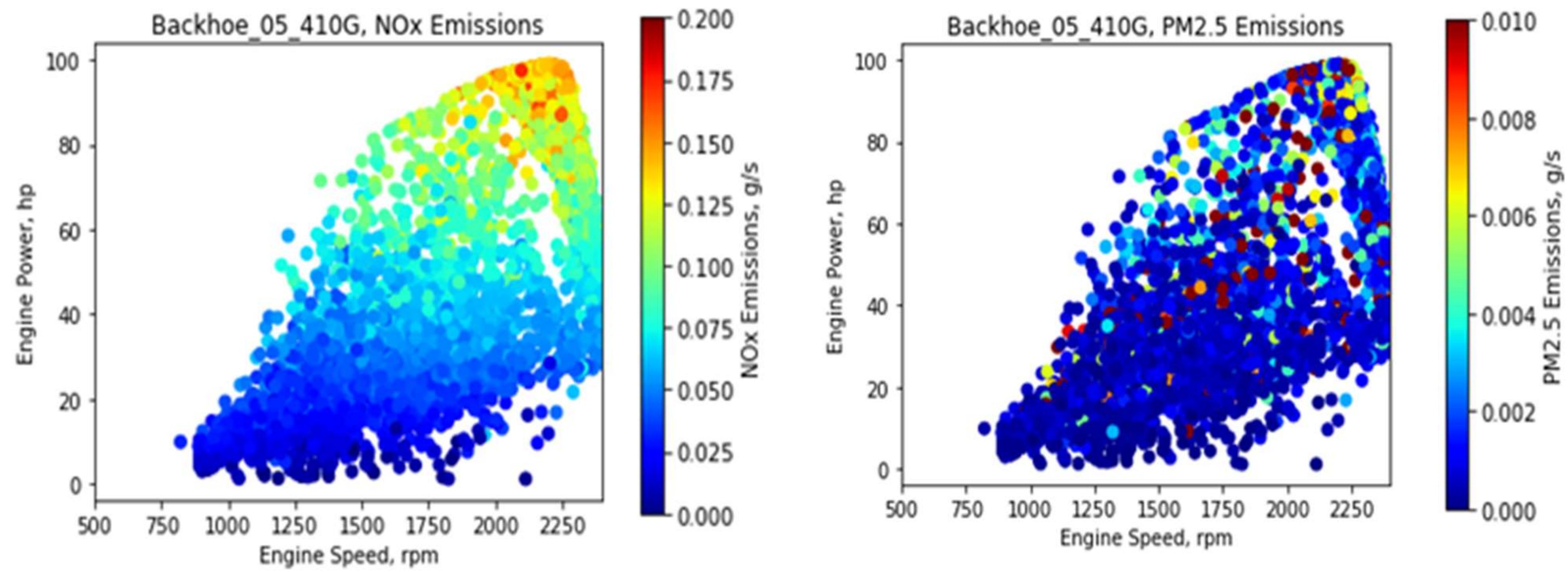
- Standard certification cycle has only select data points
- Real world data much more variable
- Need to characterize load speed patterns for various offroad vehicle/engine combinations

EPA, 2014

Emission factors and OFFROAD model



Emission rate variability with load and speed



- Plot shows sample result for a Tier 2 backhoe from 1Hz ECU and PEMS data
- Emission rates for both NOx and PM2.5 vary by more than an order of magnitude
- Vary widely with engine power (load) and speed (rpm)
- Does it affect emission factors and current emissions assessment approach?

Gaps in OFFROAD modeling

Category	Gap	Physical significance
Emissions	Emission factors borrowed from EPA	Adaptation timeline to Standards: Low sulfur, 500 ppm. CARB 1993, EPA 2007 Ultra Low Sulfur, 15 ppm. CARB 2006, EPA 2010 Aromatic content, 10 ppm. CARB 1993, no EPA limits
	Effect of load and RPM on emissions	Emissions highly variable with both parameters
	Fuel consumption data borrowed from outdated non-CA values (MY 1988-1995)	Not representative of modern engines in CA
	Effect of hybridization technologies not assessed	Knowledge of hybridization impacts are lagging way behind on-road sector
Activity	Surrogate based load factors	Biases in emissions estimates
	Hybrid powertrains not assessed	Effect of hybridization on energy consumption not understood

Construction equipment evaluated

Backhoe

Wheel Loader

Bulldozer

Excavator

Scraper

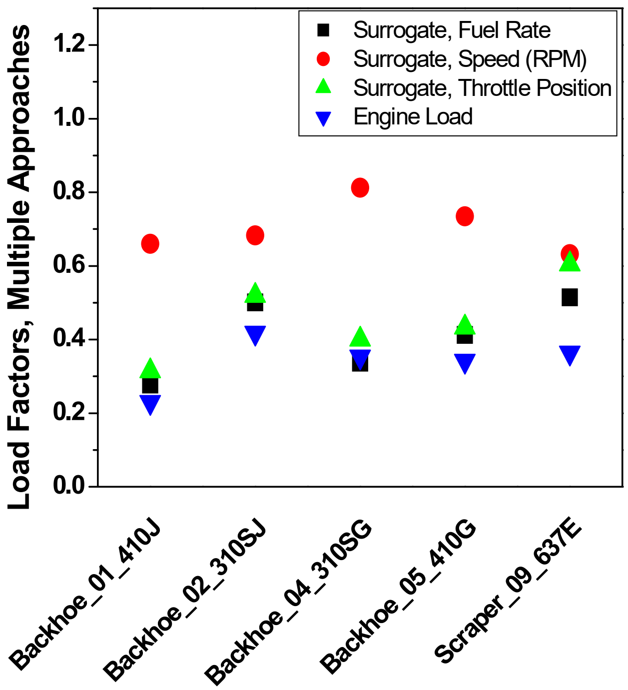
Grader

Equipment details

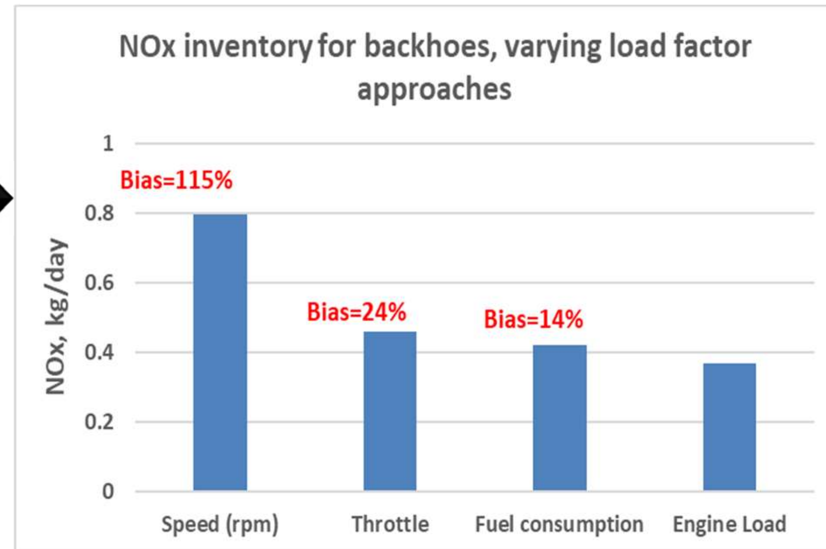
Equipment	Power (hp)	Numbers tested				Model Year	Active hours
		Tier 1	Tier 2	Tier 3	Tier 4i		
Backhoe	92-99		3	1		2006-'10	242-2599
Wheel Loader	156-273		1	5		2004-'11	242-2294
Scraper	193-280		2	1		2006-'10	439-10000
Excavator	148-269			3 (1 hybrid)		2006-'12	245-5233
Grader	163-168			4 (1 DPF retrofit)		2008-'10	952-3815
Bulldozer	223-338		1		5 (2 hybrids)	2003-'12	24-17149

- ARB contract # 08-315
- Covers a wide range of equipment, model year, tiers, power rating and active hours
- Testing carried out by CE-CERT (UCR) in 2010-2012; 3-6 hrs of data collected per equipment
- Tier 4i equipment have DPFs; NOx after-treatment information is unavailable

Multiple approaches to load factor and their inventory implications



$$E_{Species,i} = EF_{Species,i} \times P_{Rated} \times LF_i \times A_i$$



- Every surrogate method is higher than engine load-based approach
- To calculate emission inventory bias:
  - **Keep constant:** emission factor (NOx EF = 3.7 g $hp^{-1}hr^{-1}$), rated power (98 HP), activity (3.1 hrs)
  - **Vary:** load factor (based on multiple approaches)

How does hybridization affect load factors?

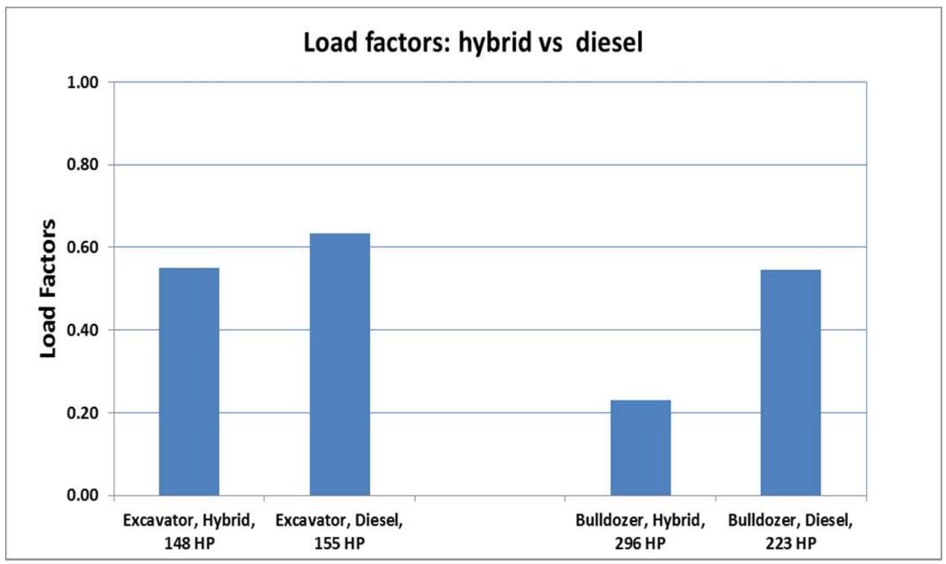
$$\mathrm{LF}_{\mathrm{Avg}} = \frac{\sum_{S=1}^{N_S}\sum_{p=1}^{N_P} \left(\text{\% Activity}\right) \times \left(\text{Load in each bin}\right)}{P_{Rated}}$$

% Activity

% Load	% Speed				
	0-20	20-40	40-60	60-80	80-100
0-20		0.2180	0.0156	0.0016	
20-40	0.0004	0.0251	0.0486	0.0107	
40-60		0.0089	0.0899	0.0917	
60-80		0.0032	0.0649	0.1306	
80-100			0.0502	0.2405	

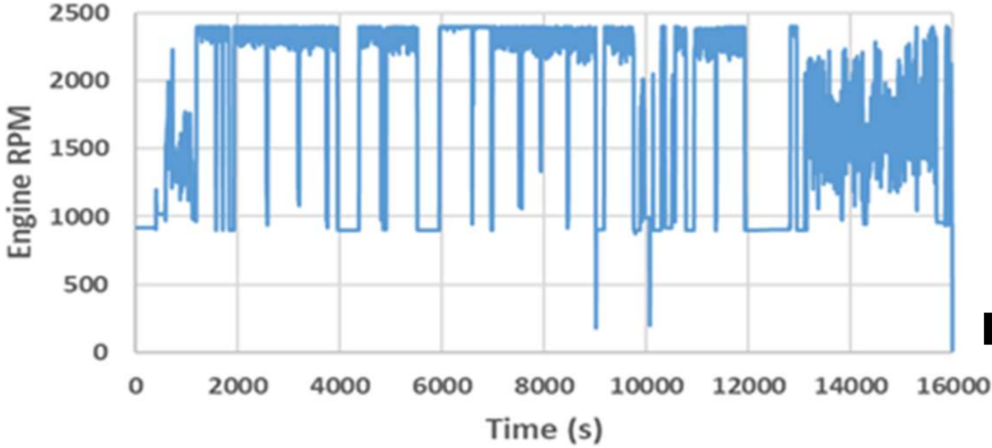
Load in each bin

% Load	% Speed				
	0-20	20-40	40-60	60-80	80-100
0-20		15.32	21.57	17.46	
20-40	36.01	41.21	47.01	46.72	
40-60		71.65	73.89	79.24	
60-80		100.04	102.61	105.79	
80-100			131.59	132.48	

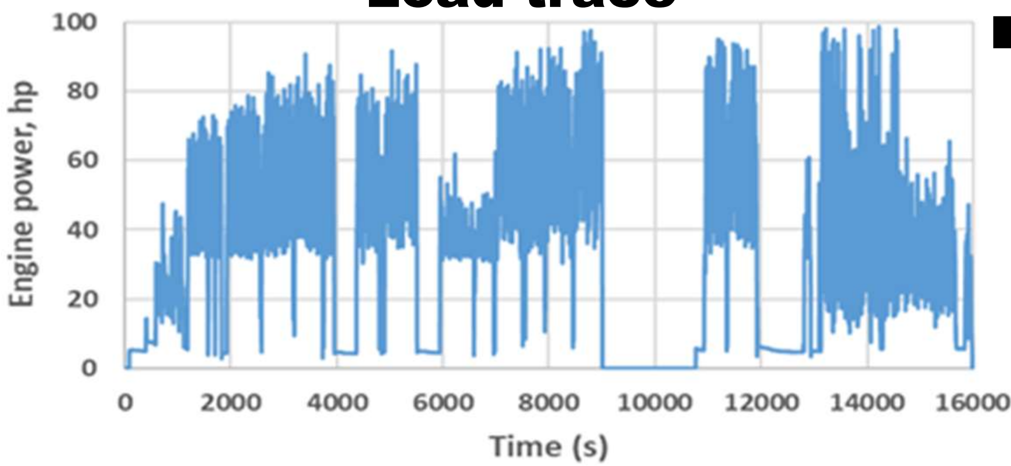


Load-RPM patterns for a sample backhoe

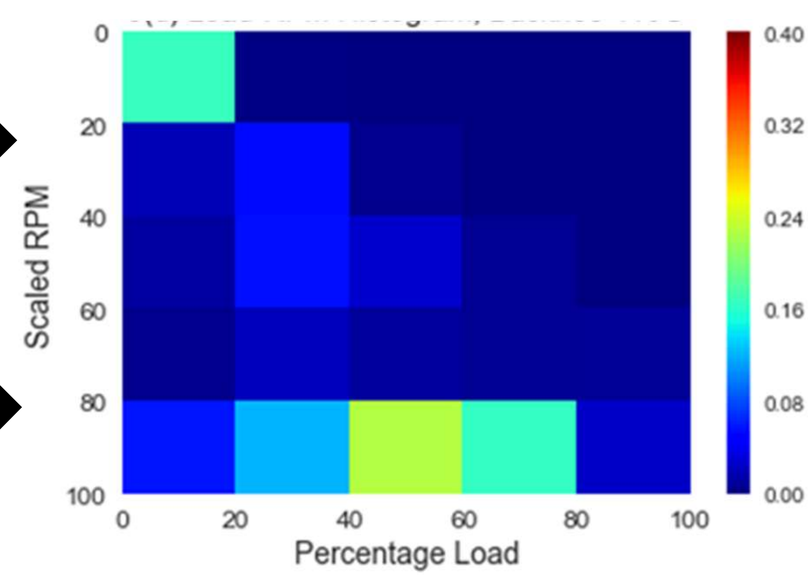
RPM trace



Load trace



Load-RPM pattern



Schematic of proposed emissions assessment

Load bins

Speed bins

$$E_{Species} = P_{Rated} \times \sum_{S=1}^{N_S} \sum_{p=1}^{N_P}$$

EF, g hp^{-1} hr^{-1}

		% Speed (RPM)				
		0-20	20-40	40-60	60-80	80-100
% Load	0-20		7.96	7.96	7.69	6.09
	20-40	6.58	5.59	5.91	5.77	5.10
	40-60	3.83	4.57	4.91	4.72	4.51
	60-80		4.28	4.15	4.05	4.24
	80-100			4.15	4.34	4.27

×

Load factors

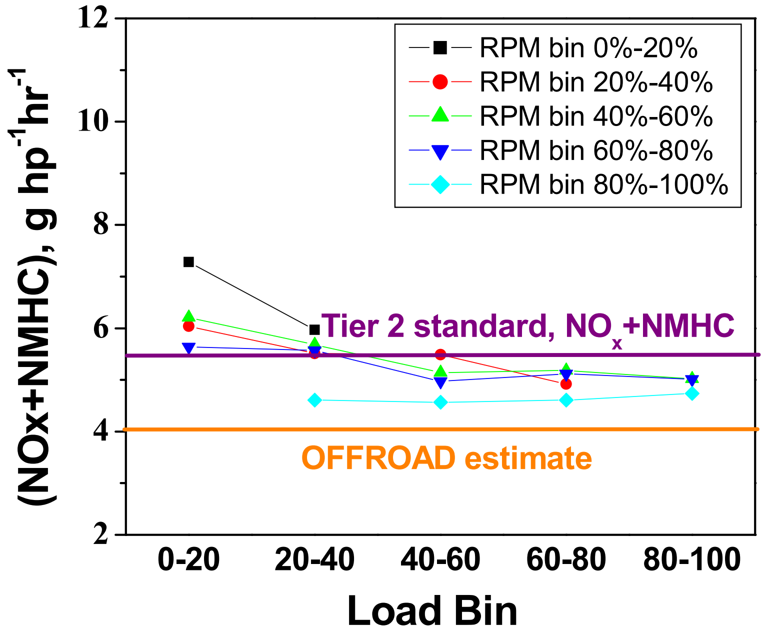
		% Speed (RPM)				
		0-20	20-40	40-60	60-80	80-100
% Load	0-20		0.14	0.13	0.14	0.17
	20-40	0.25	0.28	0.29	0.31	0.34
	40-60	0.46	0.49	0.48	0.49	0.48
	60-80		0.69	0.69	0.69	0.69
	80-100			0.84	0.84	0.84

×

Activity hrs/day

		% Speed (RPM)				
		0-20	20-40	40-60	60-80	80-100
% Load	0-20		0.095	0.076	0.012	0.023
	20-40	0.009	0.082	0.100	0.107	0.943
	40-60	0.0002	0.013	0.038	0.050	0.747
	60-80		0.002	0.010	0.019	0.238
	80-100		0.000	0.003	0.031	0.099

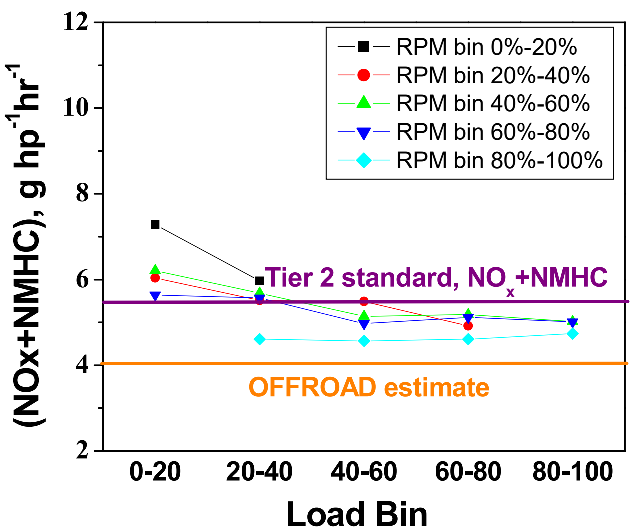
Comparison of NOx emission factors



- Load-RPM approach higher than OFFROAD for most load-RPM bins except for lowest load bins....

Comparison of NOx emission rates

Emission factors



Speed bins

Load bins

$$P_{Rated} \times \sum_{S=1}^{N_S} \sum_{p=1}^{N_P}$$

EF, g hp^{-1} hr^{-1}

		% Speed (RPM)				
		0-20	20-40	40-60	60-80	80-100
% Load	0-20		7.96	7.96	7.69	6.09
	20-40	6.58	5.59	5.91	5.77	5.10
	40-60	3.83	4.57	4.91	4.72	4.51
	60-80		4.28	4.15	4.05	4.24
	80-100			4.15	4.34	4.27

✖

Load factors

		% Speed (RPM)				
		0-20	20-40	40-60	60-80	80-100
% Load	0-20		0.14	0.13	0.14	0.17
	20-40	0.25	0.28	0.29	0.31	0.34
	40-60	0.46	0.49	0.48	0.49	0.48
	60-80		0.69	0.69	0.69	0.69
	80-100			0.84	0.84	0.84

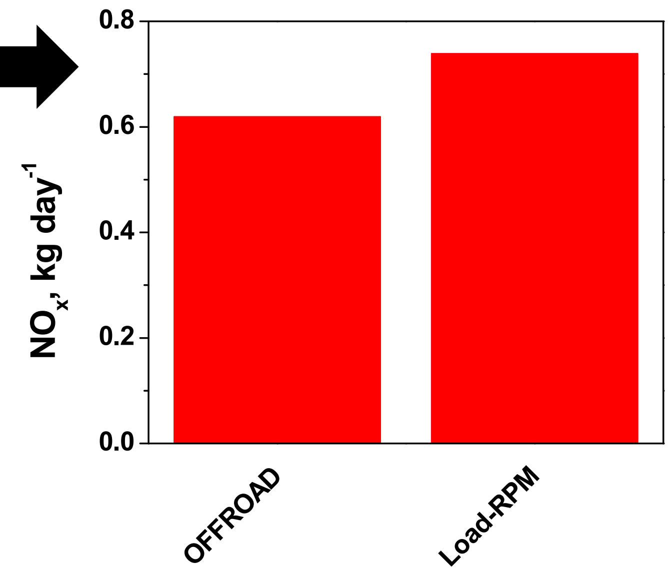
✖

Activity hrs/day

		% Speed (RPM)				
		0-20	20-40	40-60	60-80	80-100
% Load	0-20		0.095	0.076	0.012	0.023
	20-40	0.009	0.082	0.100	0.107	0.943
	40-60	0.0002	0.013	0.038	0.050	0.747
	60-80		0.002	0.010	0.019	0.238
	80-100		0.000	0.003	0.031	0.099

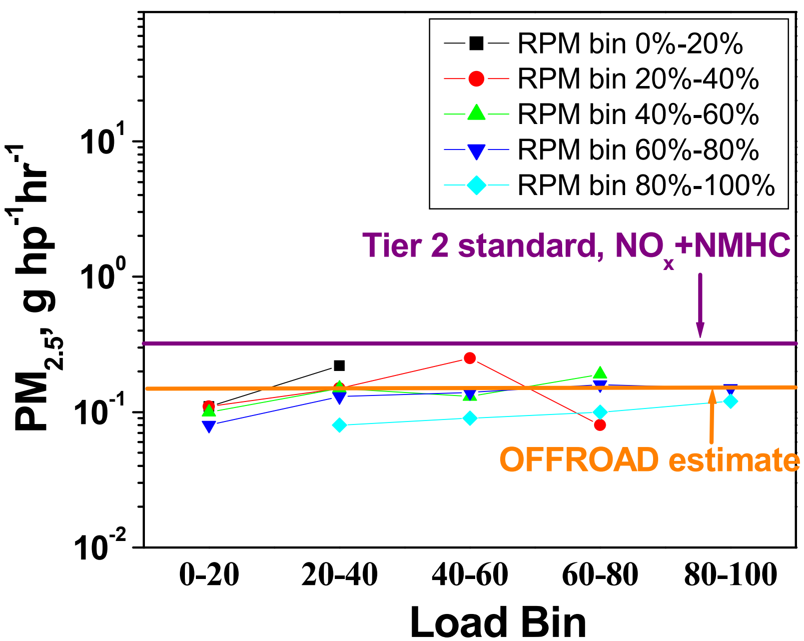
83

Overall emission rates



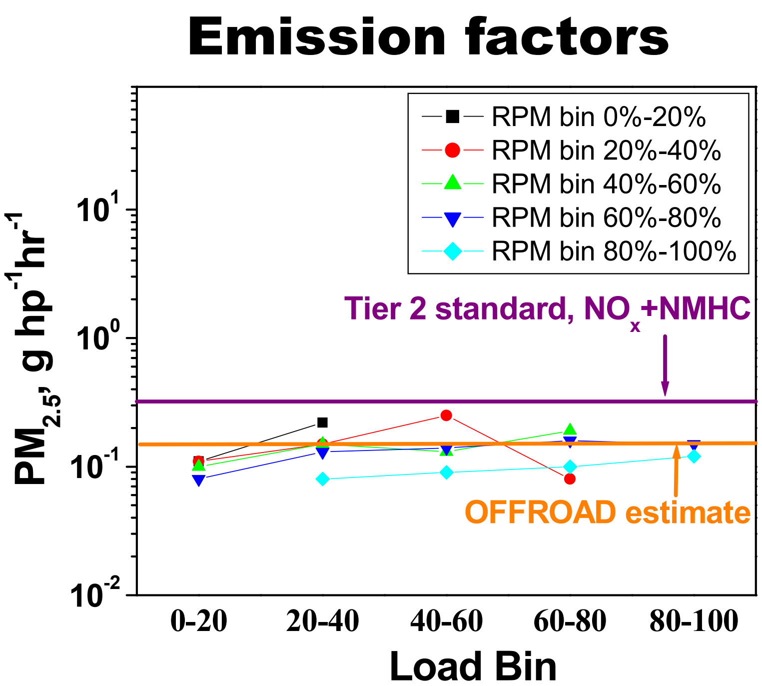
- ....resulting in higher emission rates than OFFROAD

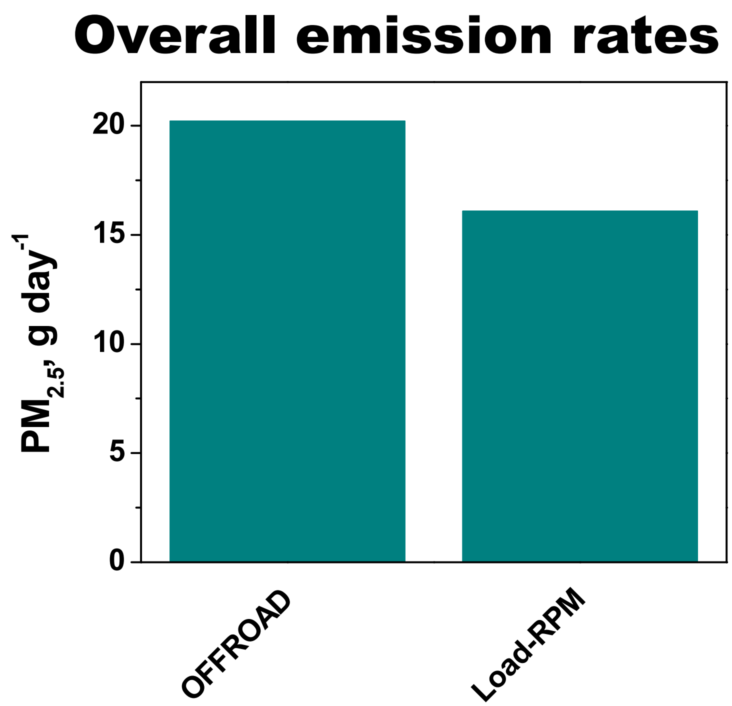
Comparison of PM2.5 emission factors



- Most load-RPM numbers are lower than OFFROAD estimates….

Comparison of PM2.5 emission rates





- ….resulting in lower emission rates than OFFROAD

What is causing higher emissions in a hybrid excavator?

Powertrain	Activity weighted values		EF (g hp^{-1} hr^{-1})	Ratio
	NOx, g hr^{-1}	Load (hp)		
Parallel hybrid	230	81	2.82	1.11
Diesel ICE	341	134	2.54	

- Decrease in engine load causing higher emissions
- PM2.5 show bigger increase with ratio of 1.4
- Similar emission trends observed for NOx emissions from hybrid bulldozers