



**Estimating Population Exposures to Toxic VOCs in Southern California
Utilizing the Community Multi-scale Air Quality Model version 5.3.2
(CMAQv5.3.2)**

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Presentation Outline

- Background – introduction and motivation
- Methods – model setup and simulation
- Results – findings and model evaluation
- Summary – take-home messages and future direction
- Acknowledgment

Background – introduction and motivation

- A toxic air contaminant (TAC) is an air pollutant which may cause or contribute to an increase in mortality or an increase in serious illness, or which may pose a present or potential hazard to human health (*Section 39655, California Health and Safety Code*).
- In the past, several air toxics programs were enacted in California such as the Toxic Air Contaminant Identification and Control Act (AB1807: Tanner, 1983) which requires the State to reduce public exposure to air toxics, and the Air Toxics Hot Spots Information and Assessment Act (AB2588: Connelly, 1987) which requires stationary sources to report the types and quantities of specific toxic pollutants their facilities routinely release into the air.
- More recently, in response to the Assembly Bill (AB) 617 (Garcia, Chapter 136, Statutes of 2017), California Air Resources Board (CARB) established the Community Air Protection Program (CAPP) with an objective to reduce exposure in communities that are most impacted by air pollution.

Methods - model setup and simulations

- In the current study, areas under two air districts in southern California were divided into two separate modeling domains. The figure below shows the extents of the modeling domains of South Coast AQMD and San Diego County APCD.



South Coast: 212x80 grid cells

San Diego: 68x70 grid cells

- These modeling domains have 2-km horizontal resolution.

Methods – model setup and simulations (Cont'd)

- Emissions – model ready speciated and gridded hourly emissions were generated by combining biogenic emissions (MEGAN), area source emissions (SMOKE) and on-road emissions (EMFAC). Point source emissions were generated during CMAQ's inline processing.
 - Two emissions scenarios: 1) GID617 which includes emissions from the USA and Mexico and 2) GID618 which includes emissions from the USA only were utilized so that contributions from Mexico emissions to toxic pollutant concentrations and total risks are estimated, particularly, in San Diego County.
- Meteorology – The meteorology was generated from the Weather Research Forecast version 3.9.1.1 (WRFv3.9.1.1) model output followed by MCIPv5.1 pre-processing. The meteorological parameters were resolved at 2-km resolution horizontally and at variably spaced 30-layers extending up to 16-km above ground vertically.
- Air Quality Model – CMAQv5.3.2 with SAPRC07tc_ae6_aq chemical mechanism and AERO7 aerosol module was applied in the current study.
- Boundary conditions – large-scale output from CAM-CHEM model simulations conducted at NCAR was used to drive the state-wide 12-km runs, and output from the 12-km runs was used as BC for the 2-km runs.
- Simulation period – January 1 to December 31, 2017.

Results

- CMAQ predicted hourly toxic VOC concentrations were first converted to daily average concentrations and later daily average concentrations were used to calculate annual average concentrations.
- Annual average concentrations were applied to calculate cancer risks at 30-year exposure level for individual toxic VOC species based on corresponding cancer potency factor and calculated risks from individual VOC were then summed to get the total toxic VOC cancer risks.
- Modeled annual/daily average concentrations of major toxic VOCs were compared to measured dataset available for 2017 to demonstrate model performance.

Major toxic VOCs considered in this study

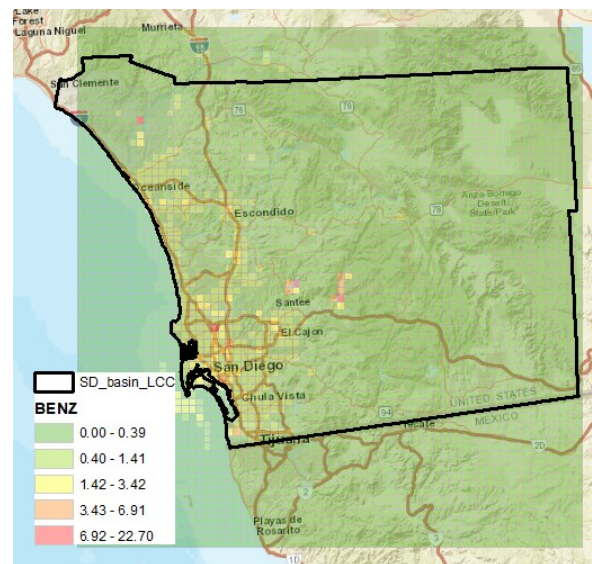
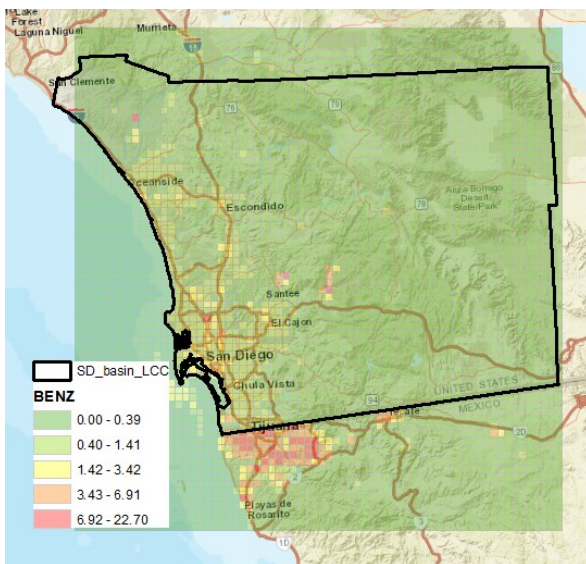
- * unit (1/(mg kg⁻¹day⁻¹))

Species	CPF* (Cancer Potency Factor)
Acetaldehyde	1.00E-02
Formaldehyde	2.10E-02
1,3-Butadiene	6.00E-01
Benzene	1.00E-01
p-Dichlorobenzene	4.00E-02
Perchloroethylene	2.10E-02

San Diego County Air Pollution Control District Modeling

Annual totals for two emissions scenarios

Toxic Air Contaminant	2017 Emissions in tons per year (tpy)	
	Emissions (USA + Mexico)	Emissions (USA)
Formaldehyde	1926	1037
Acetaldehyde	1329	926
1,3-Butadiene	286	156
Benzene	1148	551
Perchloroethylene	734	342
p-Dichlorobenzene	60	32



An Example of annual emissions of benzene (tpy)

- Left – emissions from US + Mexico
- Right – emissions from US

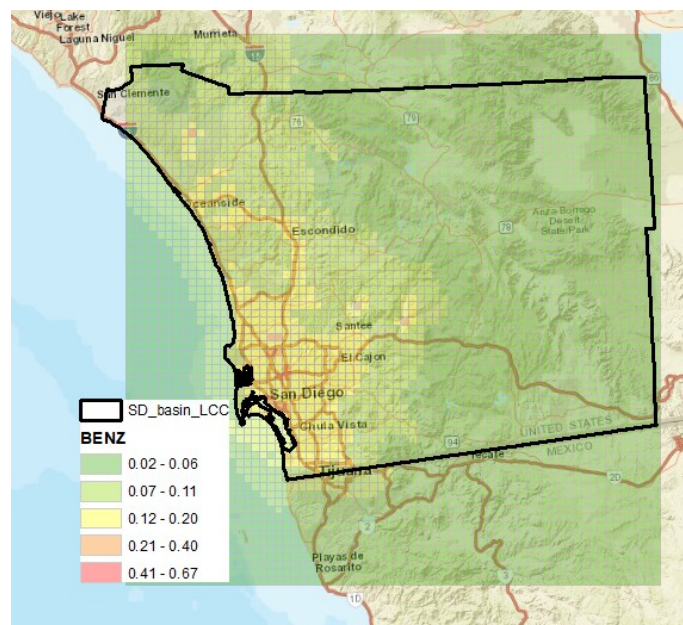
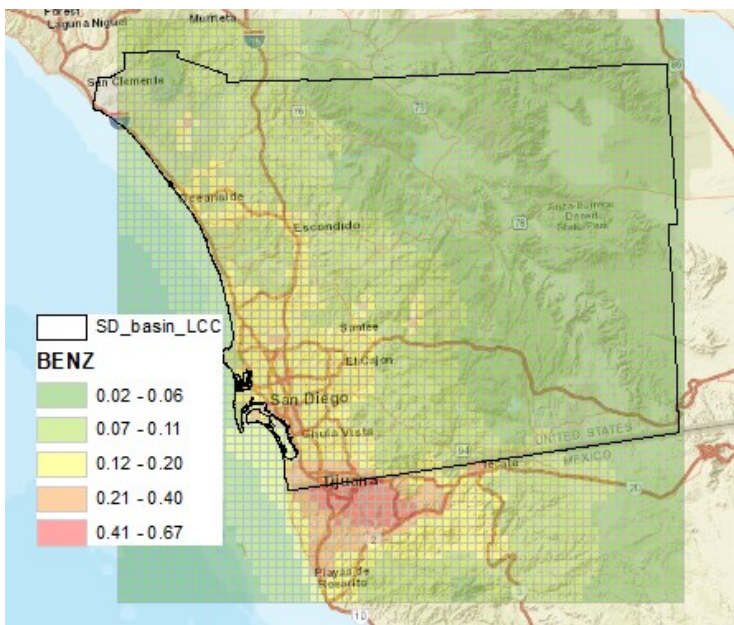
Note that benzene emissions are much higher near the border areas in Mexico compared to the adjacent areas in the US.

Annual average concentration of benzene (ppb) within the SDC modeling domain

Simulations were carried out using emissions from:

- Left - USA plus Mexico
- Right – USA only

Note that the concentrations of benzene are much higher ($\sim 2x$), particularly, in areas near the US-Mexico border. This clearly shows the impact of cross-border transport of toxic VOCs.



Population weighted 30-yr exposure level VOC cancer risk for the San Diego County (SDC) air basin in 2017

Emissions from outside the US could contribute ~10% to the total cancer risk from toxic VOCs in the San Diego County. However, the contribution from emissions outside the US could be much higher in communities along the US-Mexico border. Also, note that the emission estimates in Mexico are highly uncertain, which will also translate to uncertainty in the risk estimates.

	Risk (per million)		
	Emissions from US and Mexico	Emissions from US only	Contributions from Mexico Emissions
VOC Air Toxics			
Formaldehyde	22.0	20.5	1.5
1,3-Butadiene	34.7	30.8	3.9
Benzene	32.4	28.6	3.8
Acetaldehyde	6.4	5.8	0.6
p-Dichlorobenzene	0.9	0.8	0.1
Perchloroethylene	4.0	3.4	0.6
Total VOC Risk	100.4	89.9	10.5

Secondary formation of toxic VOCs

- Secondary formation of acetaldehyde and formaldehyde in the atmosphere through chemical transformation contributed to ~70% of the total individual cancer risk for both VOCs in San Diego County.

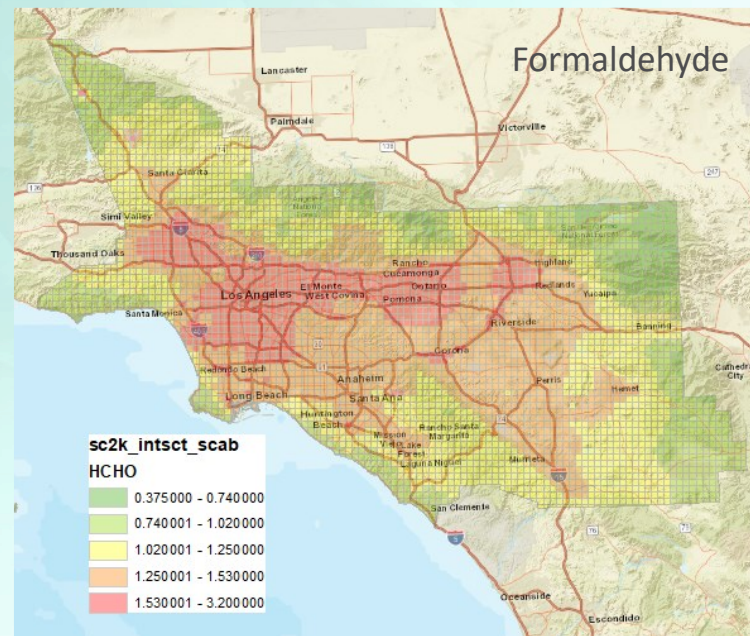
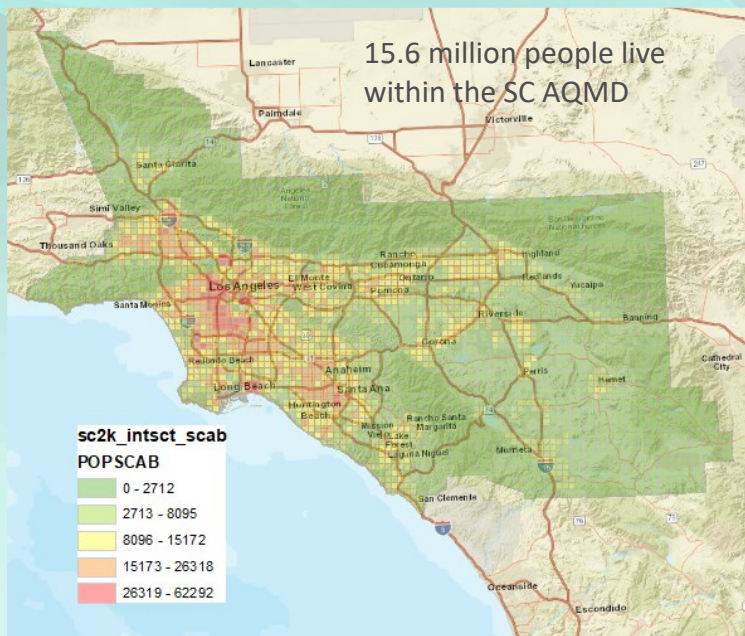
Contributions to 30-yr exposure cancer risk (%)

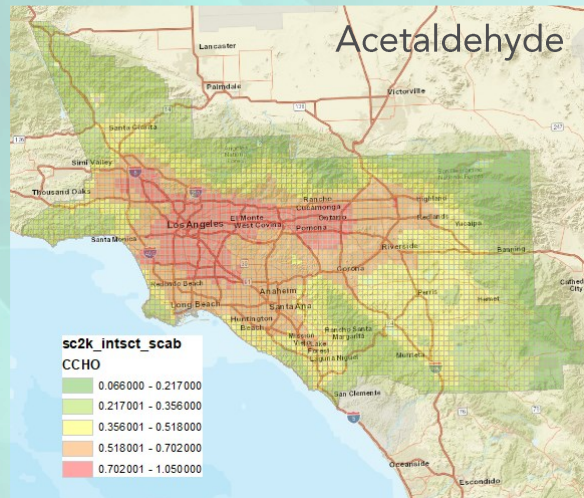
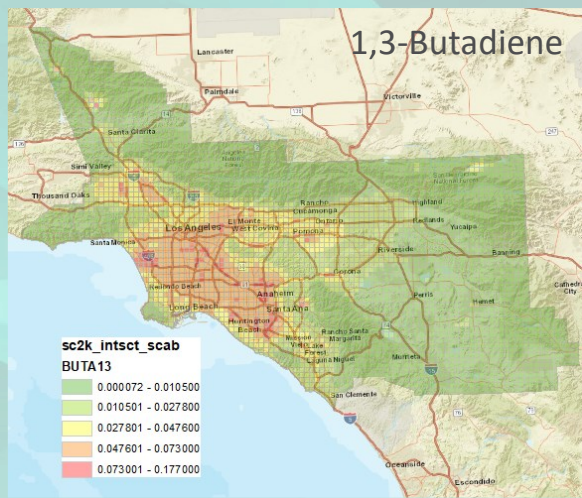
Emissions (USA + Mexico) Emissions (USA)

Toxic VOC	Primary	Secondary	Primary	Secondary
Formaldehyde	31	69	28	72
Acetaldehyde	33	67	32	68

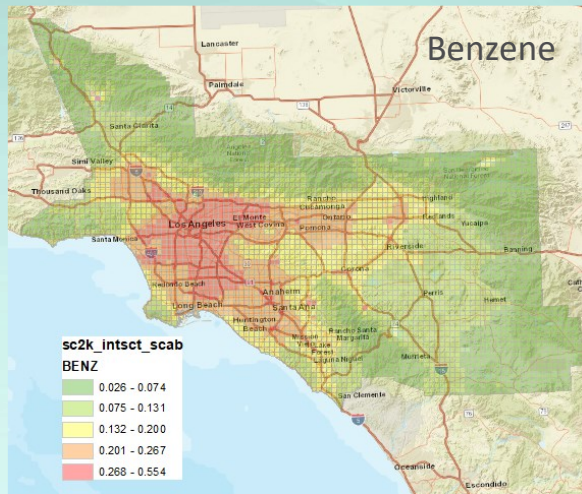
South Coast Air Quality Management District Modeling

Distributions of population (2010 census) and annual average concentrations (2017) of toxic VOCs within South Coast Air Basin





Plots of 2017 annual average concentrations (ppb) of toxic VOCs



Toxic VOC species	Population weighted annual average concentration (ppb) in SoCAB
Acetaldehyde	0.65
Benzene	0.23
Formaldehyde	1.51
1,3-Butadiene	0.04
p-Dichlorobenzene	0.01
Perchloroethylene	0.07

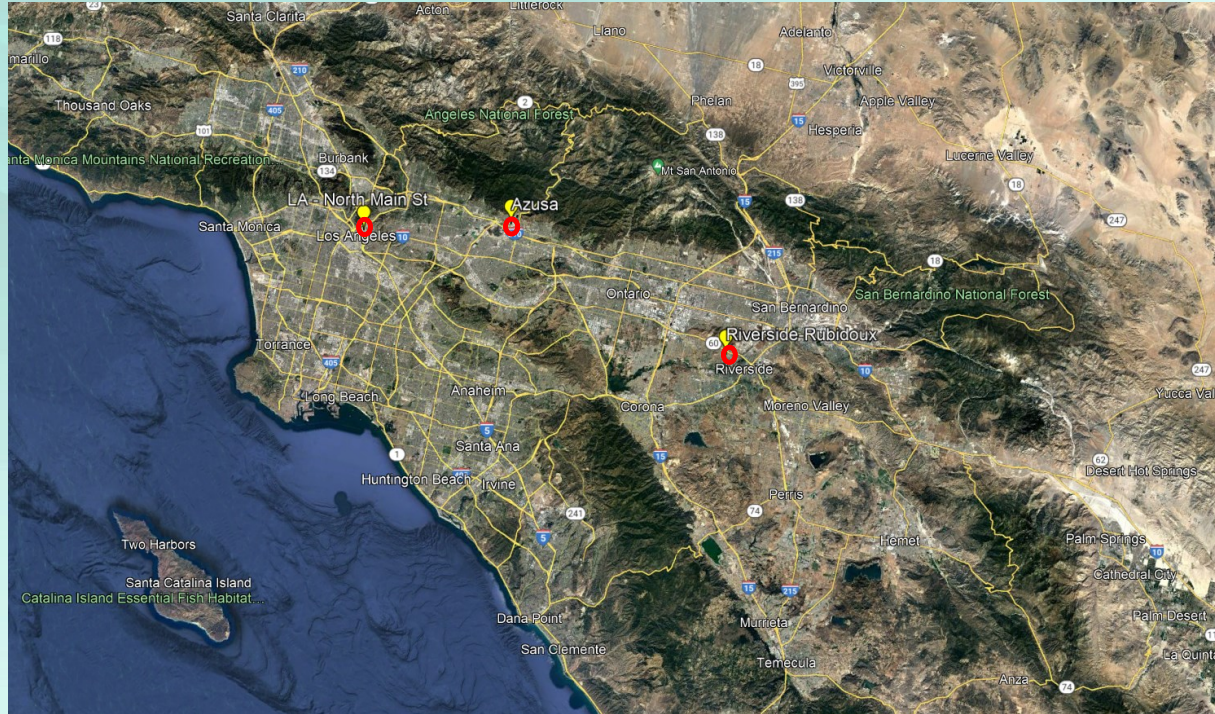
Population weighted 30-yr exposure level VOC cancer risk for the South Coast air basin in 2017

Toxic VOC species	Risk (per million)
Formaldehyde	26.3
1,3-Butadiene	36.9
Benzene	49.4
Acetaldehyde	8.0
p-Dichlorobenzene	1.4
Perchloroethylene	6.9
Total VOC Risk	128.9

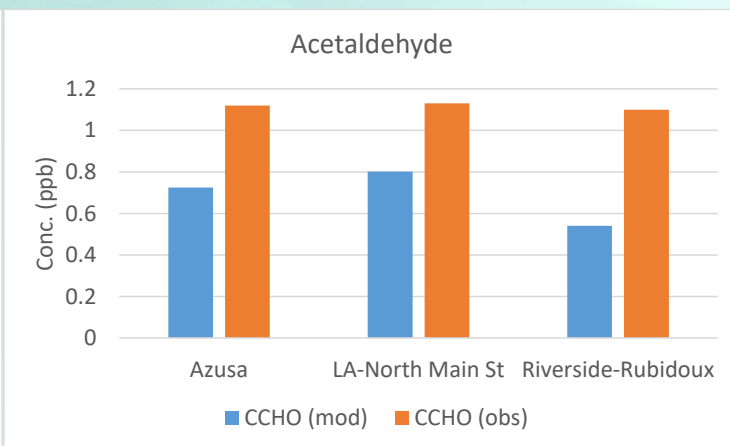
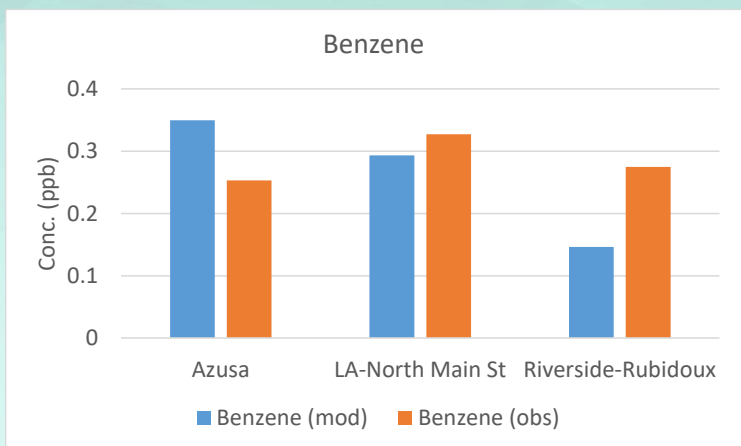
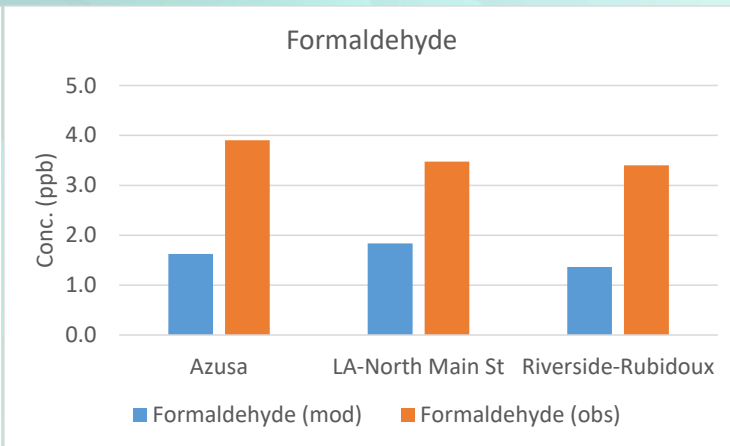
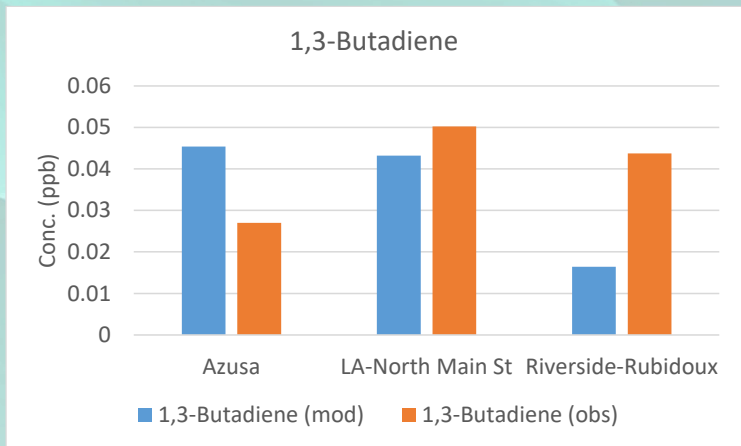
Model Performance

- Measured data were obtained from CARB's toxic VOC database.
- Only three PAMS/SLAMS sites within the South Coast AQMD modeling domain reported measured data for major toxic VOCs species in 2017. The sites are Azusa (#2484), LA-North Main St (#2899), and Riverside – Rubidoux (#2596). The data were reported typically in every 6 days.
- Model performances in predicting concentrations of total PM_{2.5}, elemental carbon (EC), and 8-hr Ozone were also carried out for several sites in the SCAQMD, but findings are not discussed here.

Location of monitoring sites reporting toxic VOCs data for 2017 within SoCAB



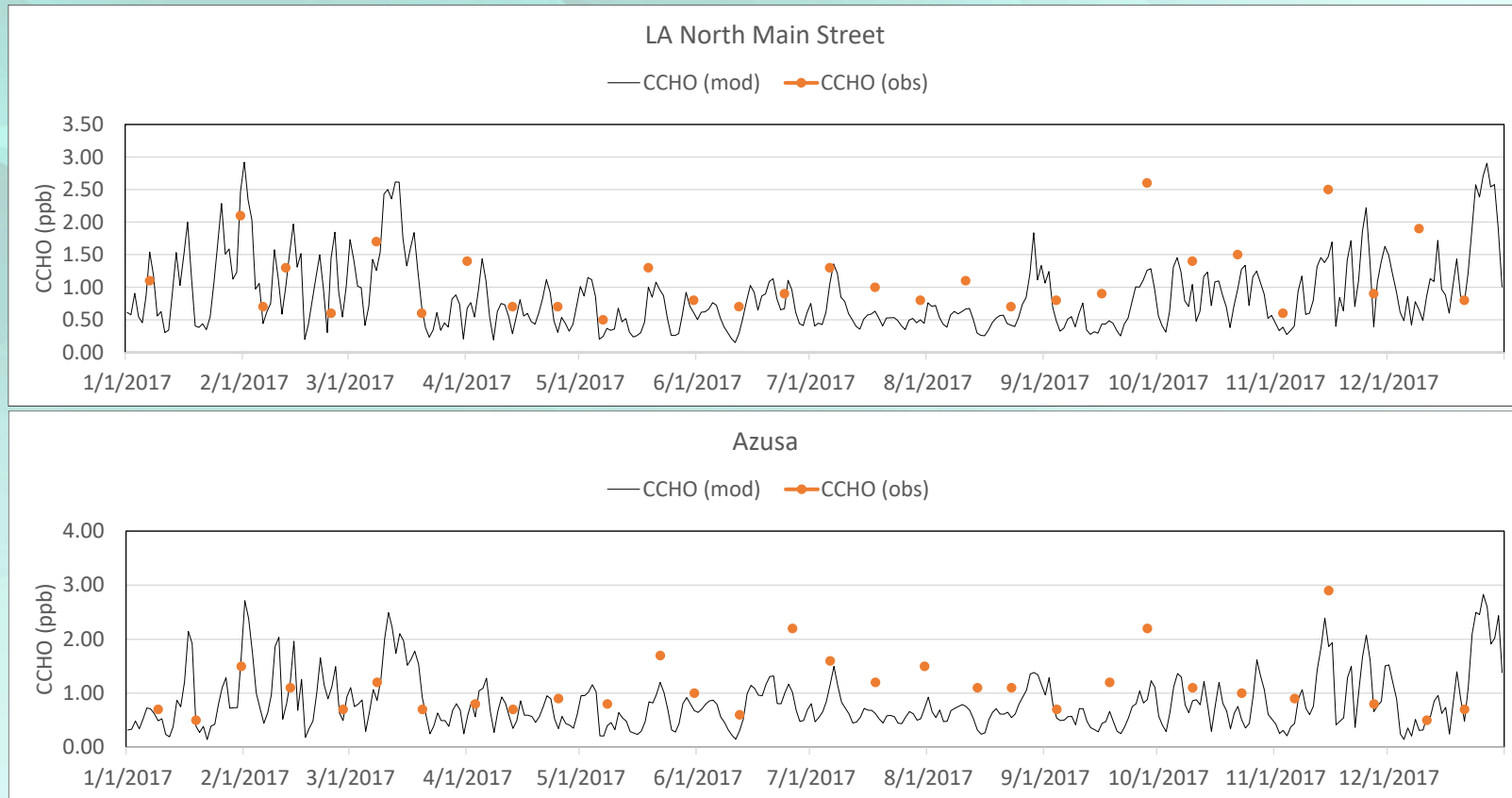
Modeled vs observed annual average concentrations of toxic VOCs in 2017



> Toxic VOCs concentrations are predicted relatively better at the LA-North Main St site compared to other two sites within SoCAB.

> The model predicted formaldehyde concentrations much lower than observed at all three sites. Column integrated modeled concentrations will be further compared to satellite data in a future effort to evaluate the model performance.

Example - time series of 24-hr averaged modeled vs observed concentrations of acetaldehyde



Summary

- Toxic VOC air quality modeling for the South Coast and San Diego County air basins in southern California have been completed for 2017 emissions.
- Secondary formation of toxic VOCs in the atmosphere such as formaldehyde and acetaldehyde could contribute as much as ~70% of the total mass concentrations.
- Communities near the US-Mexico borders are likely to be impacted more by toxic VOCs emissions from the other side of the border and that contribute as much as ~10% to the total 30-yr exposure cancer risk due to inhalation exposures to toxic VOCs.
- The CMAQv5.3.2 performed relatively well in predicting toxic VOC concentrations compared to available measured data for 2017 within the modeling domains. Other sources (e.g., satellite) of observed data as they become available will be compared to modeled data for southern California domains to demonstrate model performance in future efforts.
- Toxic VOC air quality modeling is also under way for San Joaquin Valley and northern California domains.

Thank you!

Acknowledgement: The content is solely the responsibility of the authors and does not necessarily represent the views of California Air Resources Board.