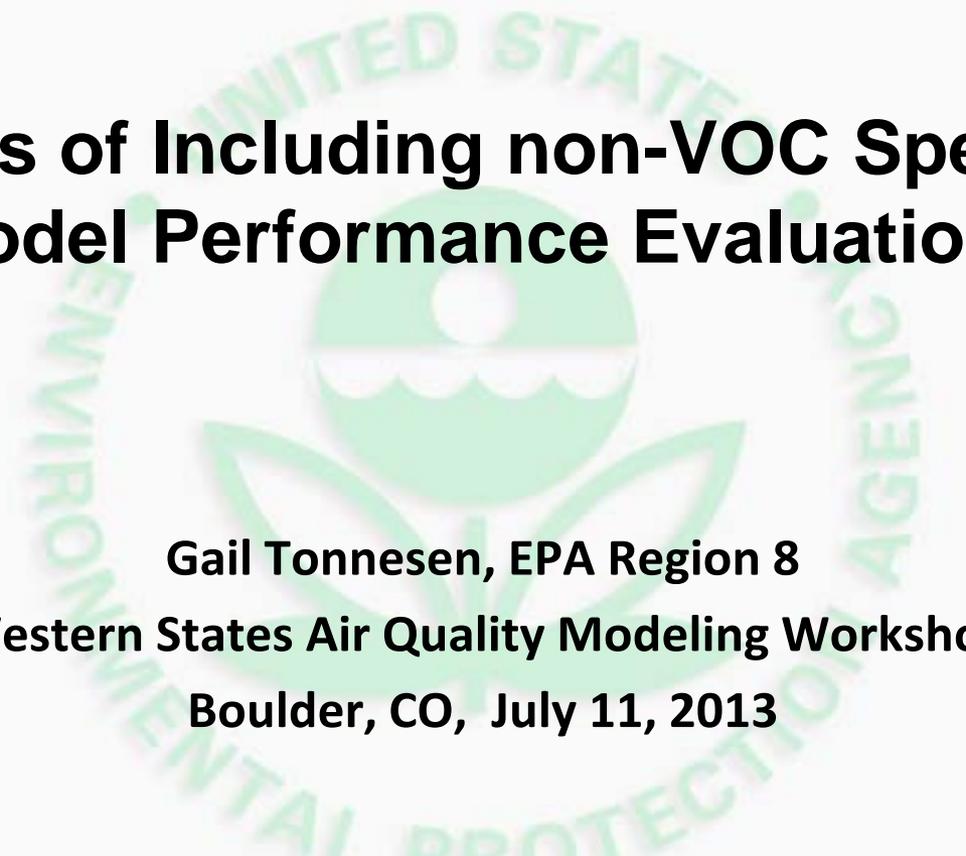




Benefits of Including non-VOC Species in Model Performance Evaluations



**Gail Tonnesen, EPA Region 8
Western States Air Quality Modeling Workshop
Boulder, CO, July 11, 2013**



Definition of VOC

- Species less reactive than ethane can be excluded from the definition of VOC:
 - current exempt list includes methane, ethane and other negligibly reactive species:
http://www.epa.gov/ttn/naaqs/ozone/ozonetech/def_voc.htm
- These exempt species are not regulated as O₃ precursors.
- Modeling methane either implicitly or explicitly does not change the status of methane and ethane as an exempt compounds for ozone control.

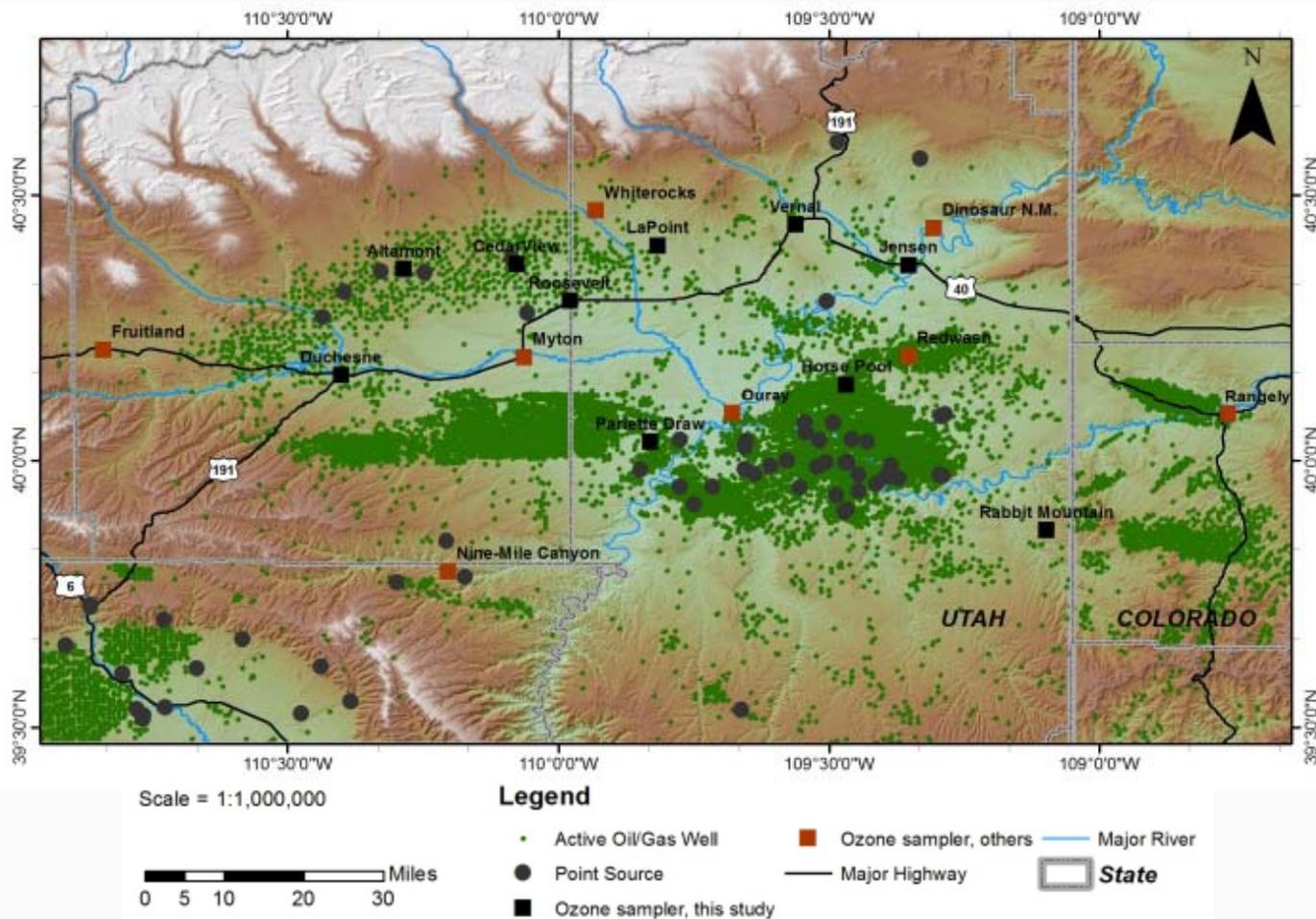


Current Modeling Approach for Methane

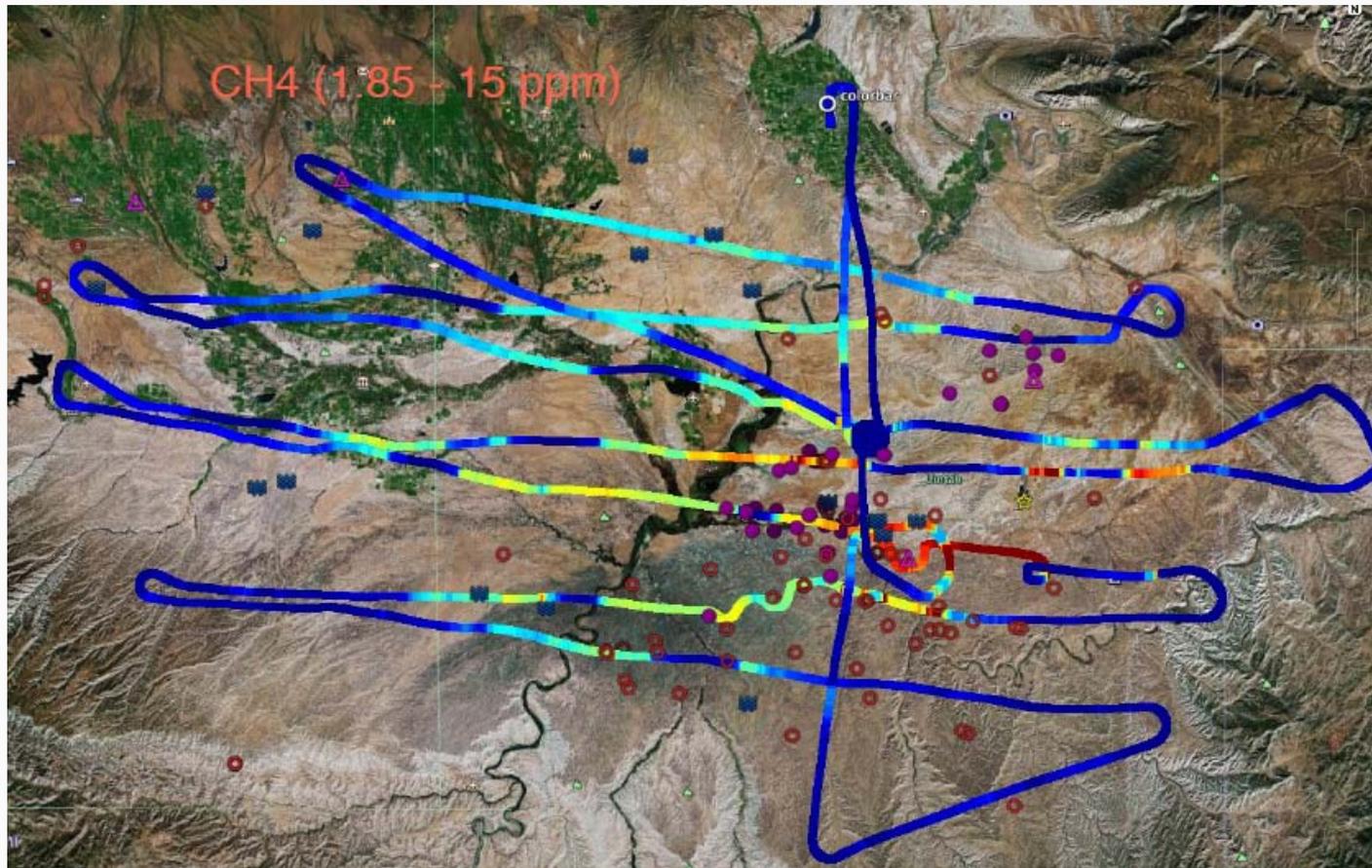
- Current practice is to model methane as a psuedo-first order reaction using constant background concentration: 1.87 ppm in 2013: $\text{OH} = \text{CH}_3 + \text{H}_2\text{O}$ (rate constant x background CH_4)
- Global methane lifetime estimated to be about 12 years, but it varies depending on local temperature and OH. At 0 C and 1 atm:
 - $\text{OH} = 1 \times 10^6$ molec/cm³: 26 years
 - $\text{OH} = 5 \times 10^6$ molec/cm³: 5 years
 - Approximately 0.01 to 0.05% of methane reacts per day, or between 0.2 to 1 ppb assuming default background CH_4 .
 - Given it's low reactivity, CH_4 can be used as a non-reactive tracer of local emissions sources.

Locations of O&G emissions sources

Figure 2-2 from Page 22, EDL 2011 Report



CH₄ concentration builds during multi-day winter inversions
Observed methane concentrations > 10 ppm



preliminary 2013 UBOS data



Value of methane observations

- Provides a tracer of vertical mixing and dispersion.
- Useful for WRF and air quality model performance evaluations.
- Observed ratio of VOC_i/CH_4 can be compared to modeled ratios to evaluate emissions inventories.
- Need to model CH_4 explicitly to evaluate model transport and emissions inventories.



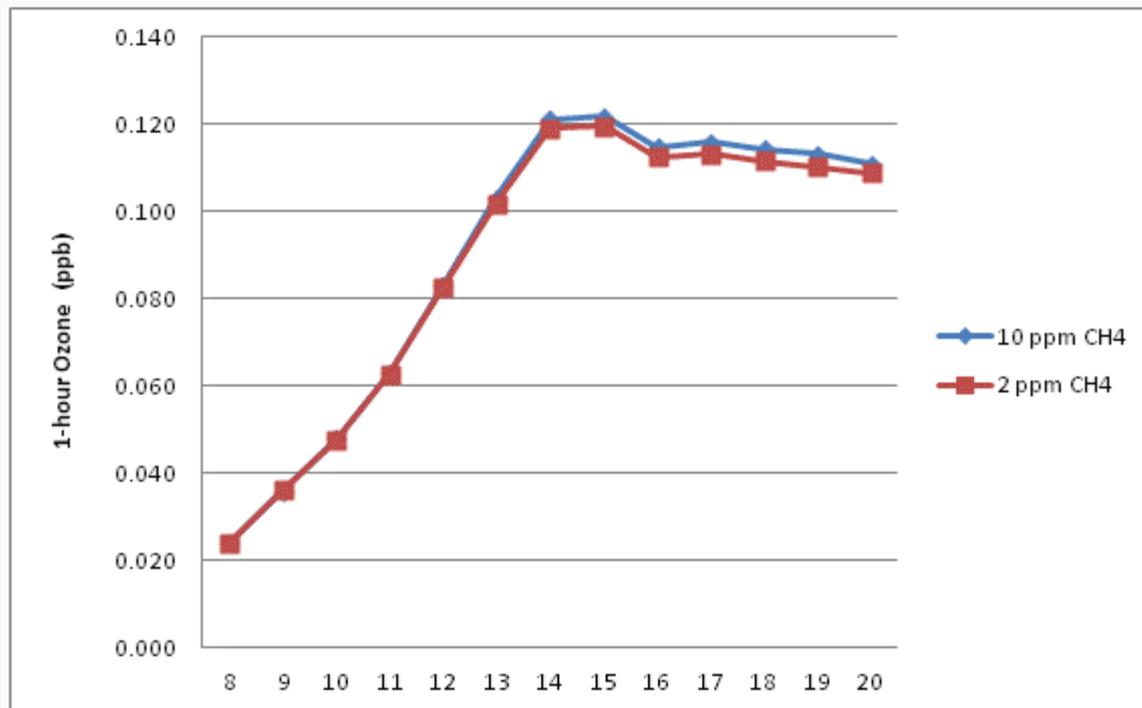
Contribution to Ozone

- Observed concentrations of methane of 10 ppm could contribute between 1 to 5 ppb ozone production per day.
- Contribution is cumulative during multiday stagnation events.
- While methane and ethane are not regulated as ozone precursors, control of VOC emissions will result in collateral reductions in methane and ethane emissions:
 - benefits of VOC control will be underestimated if methane and ethane are not explicitly included in model simulations.



Box Model Sensitivity to Methane

- Increase background CH₄ from 2 ppm to 10 ppm
- 1-hr max and 8 hour average ozone each increase by 2 ppb





Next Steps

- Data on CH₄ emissions are already available in WRAP Phase III oil and gas emissions inventories.
 - CH₄ emissions data are not written to emissions files because CMAQ and CAMx use global background CH₄.
- EPA ORD asked WRAP to include CH₄ in emissions files to aid in performance evaluation of WRF, CMAQ and CAMx:
 - we can treat CH₄ as a non-reactive tracer to aid in evaluation of dispersion and emissions, and
 - we can use explicit methane chemistry to model methane contribution to ozone.



Approach

- Continue to use default background CH₄ to represent non-local sources:
 - because CH₄ is long-lived, this approach is more accurate and less effort than modeling global CH₄ sources.
- Add explicit CH₄ only for local sources that are sufficiently large to have a measureable signal above background CH₄.