NO_2 Modeling Techniques

12th Modeling Conference on Air Quality Modeling

Chris Owen

US EPA/OAQPS/AQAD

Air Quality Modeling Group

Tiered NO_2 screening modeling

- Final Appendix W 3-Tiered screening for NO_2:
  - Tier 1 – "full conversion", all NO_X as NO_2
  - Tier 2 – Ambient Ratio Method 2 (ARM2)
  - Tier 3 – Ozone Limiting Method (OLM) and Plume Volume Molar Ratio Method (PVMRM)
- Defining "screening techniques" – Section 4.2.1.d:

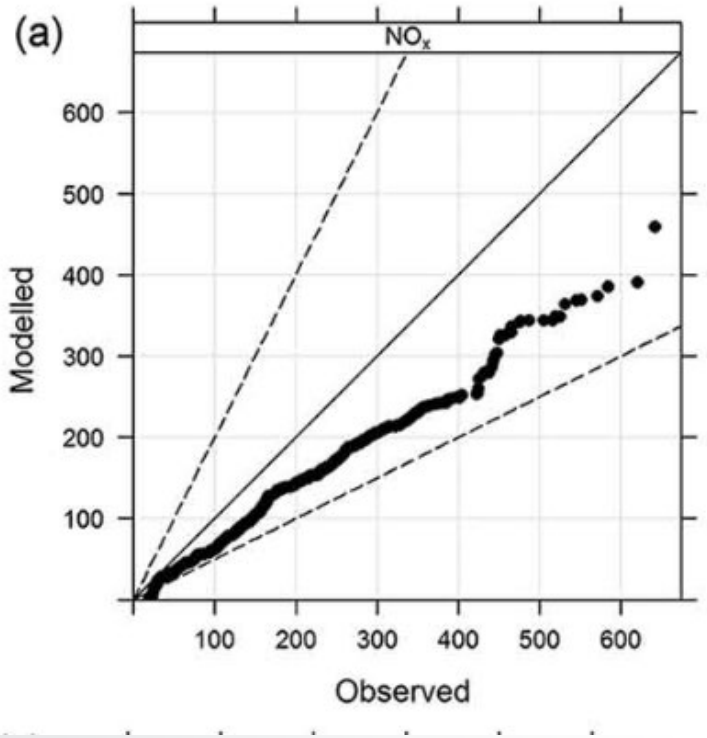
  "These screening techniques are part of the EPA's preferred modeling approach for NO_2 and do not need to be approved as an alternative model. However, as with other screening models and techniques, their usage shall occur in agreement with the appropriate reviewing authority (paragraph 3.0(b))."

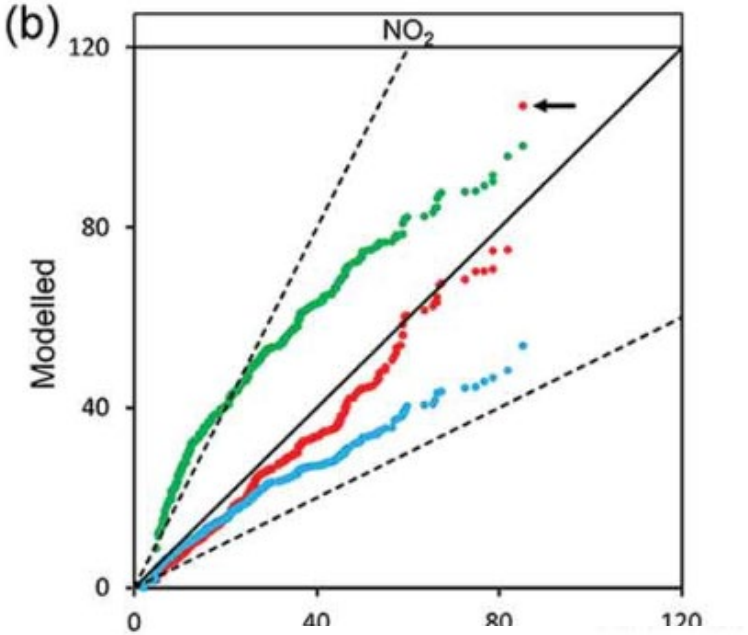
NO_2/NOx in-stack ratios update

- New data added to the EPA ISR database:
  - https://www3.epa.gov/scram001/no2_isr_database.htm
- Report and data available from PRCI member survey
  - Summary of NO_2-NO_X Ratio Test Data Compilation for Reciprocating Engines and Combustion Turbines
  - https://www.prci.org/Research/CompressorPumpStation/2792/CPS-11-2/3217/56291.aspx
  - Data will be added to the website next week
- Report available from EPRI member survey
  - Assessment of NO_2/NO_X Ratios at Fossil Fuel Power Plants
  - https://www.epri.com/#/pages/product/3002017300/?lang=en-US
  - Report is free, data will be added to the website in a few weeks

New Tier 3 Model Development

- API working with CERC to implement a version of the ADMS NO_2 scheme in AERMOD
  - Atmospheric Dispersion Model Method (ADMSM)
- Similar to PVMRM in that it accounts for plume volume and considers entrainment of ozone
  - Further limits ozone due to competition between plumes by using a plume cross-sectional area entrainment method
  - Adds “postchemistry” equilibrium calculation, i.e., conversion of NO_2 back to NO based on solar radiation
  - Computation incorporates background NO_X and NO_2 concentrations

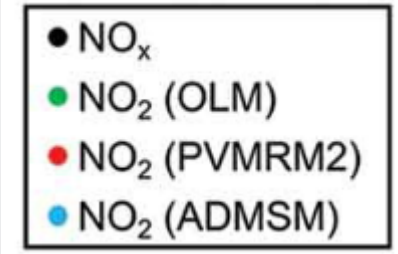


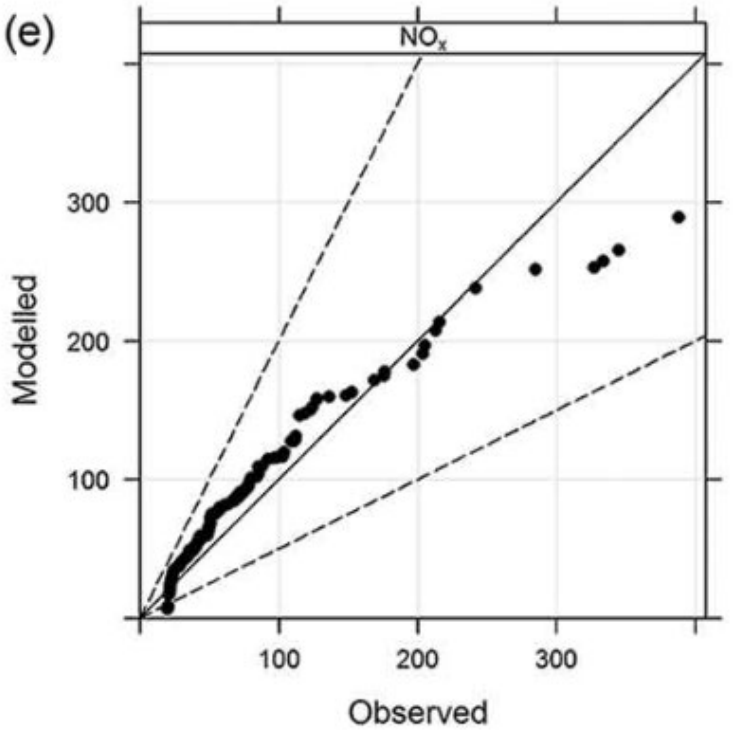


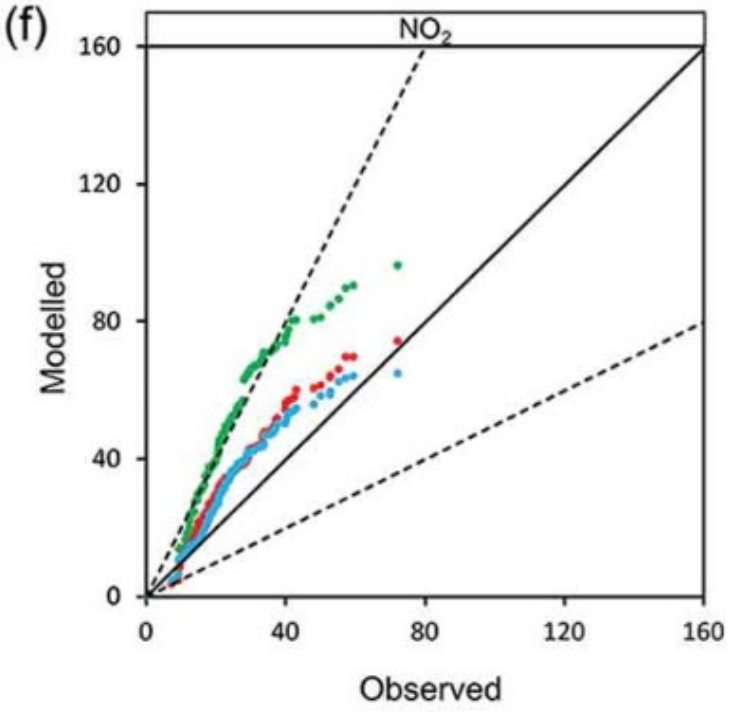
Results from Carruthers, et al, (2017) Evaluation of an explicit NOx chemistry method in AERMOD, JAWMA, 67:6, 702-712, DOI: 10.1080/10962247.2017.1280096

Empire Abo South Dataset

Palaau NO_2 dataset







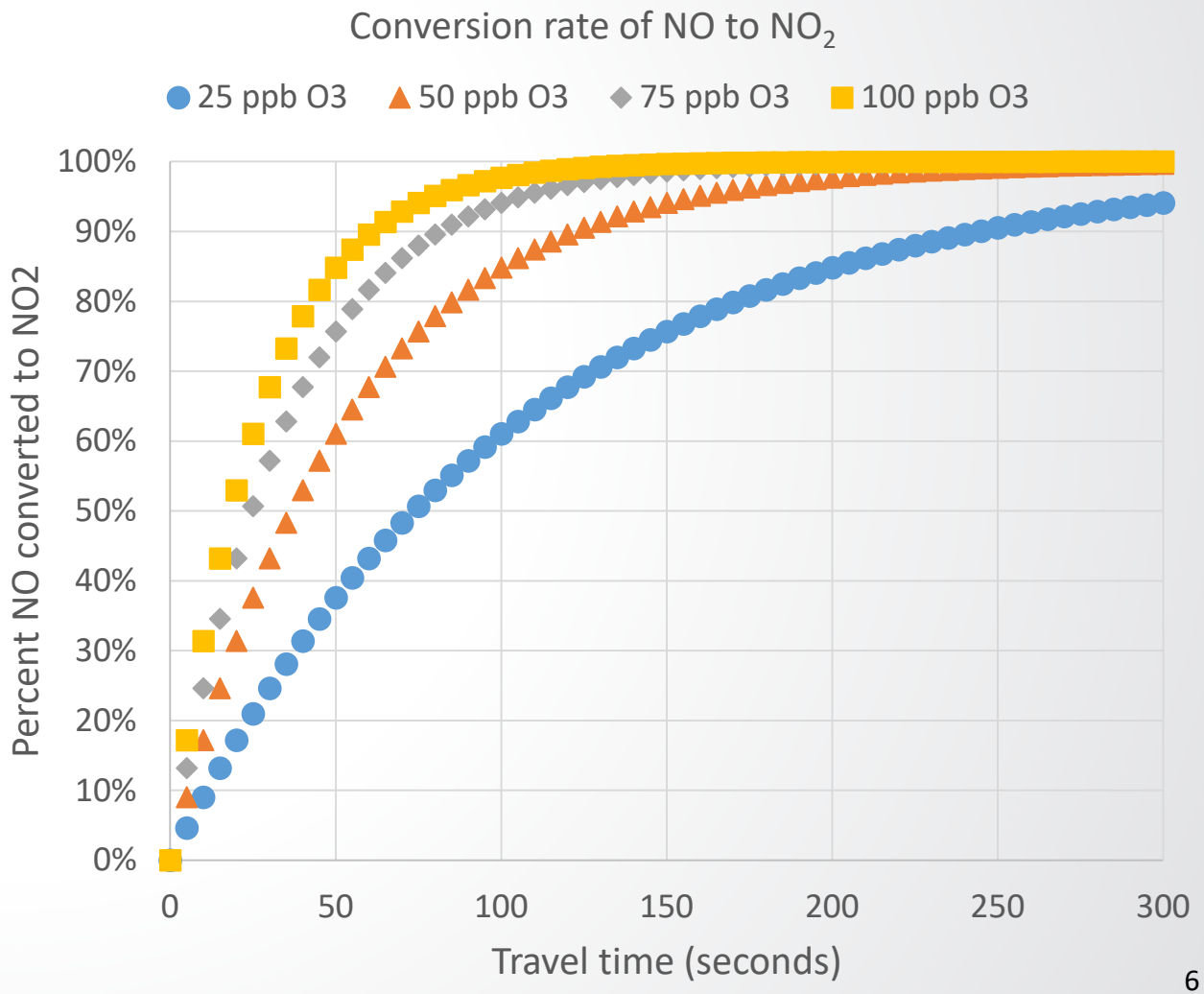
New Tier 2 Method Development

- EPA is considering a Tier 2 method based on reaction rate limitations of conversion of NO to NO_2
  - The reaction between NO and O_3 can take several minutes to reach equilibrium, based on the O_3 and initial NO concentrations:

$$[NO] = [NO]_o \exp(-k1[O_3]t)$$

  - Reaction can be bounded by the equilibrium ratio of NO_2 and NO_X, by applying the pseudo-steady state (PSS) approximation:

$$[NO_2]/[NO_X] = (k1[O_3])/(k2 + k1[O_3])$$

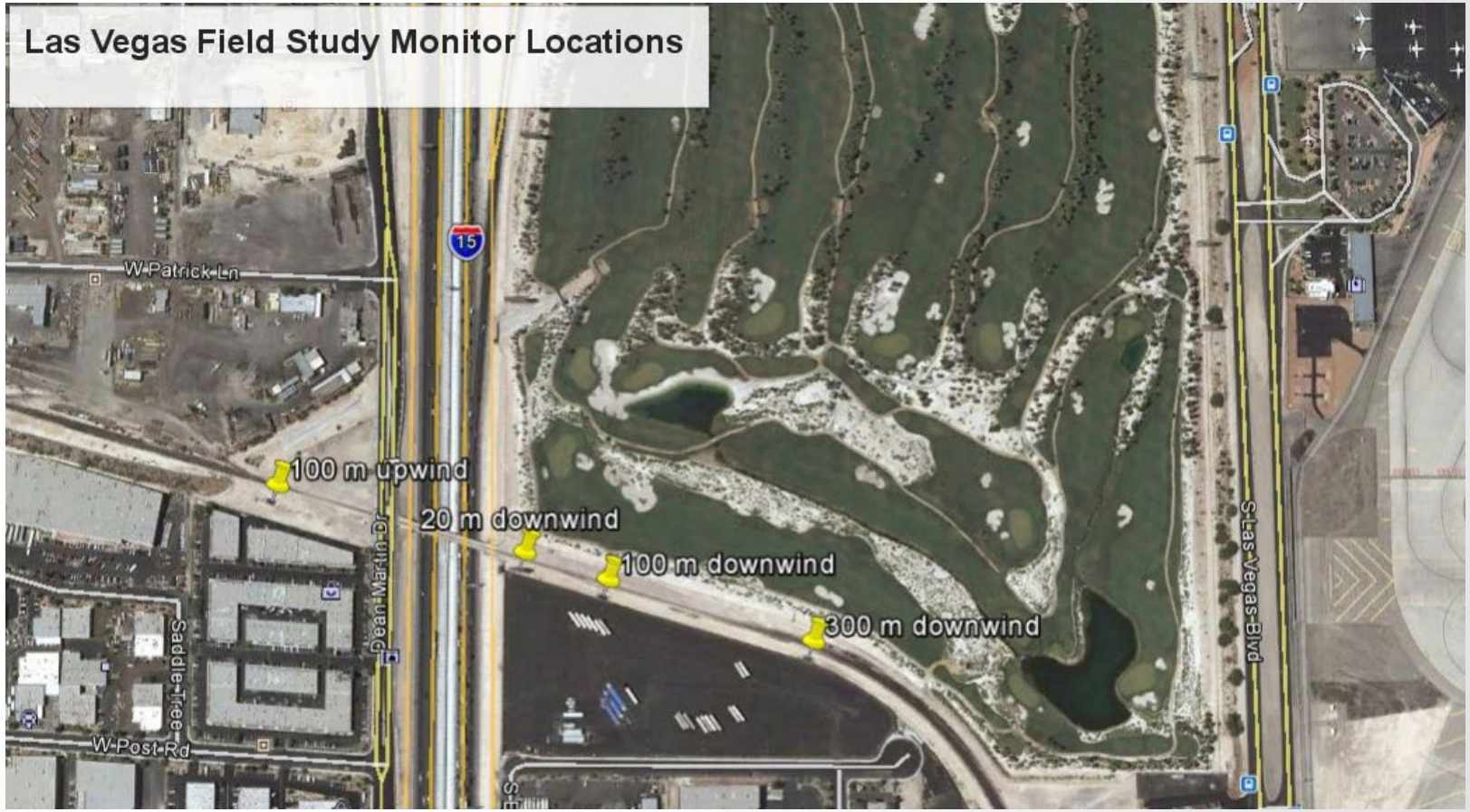


Evaluation database development

- Near-road
  - Las Vegas, Nevada
  - Detroit, Michigan
- Stationary sources
  - Denver-Julesburg Basin, Colorado Drill Rig
  - Oklahoma Compressor Station

Las Vegas field study

- Field measurements conducted from Dec 2008 – Jan 2010
- Continuous measurements of CO, NO_X, BC, PM_{10}, $PM_{2.5}$, winds, RH
- Monitoring 100 m west of the roadway and at 20, 100, and 300 m east of the roadway.
- On-site traffic monitoring, vehicle counts in each lane



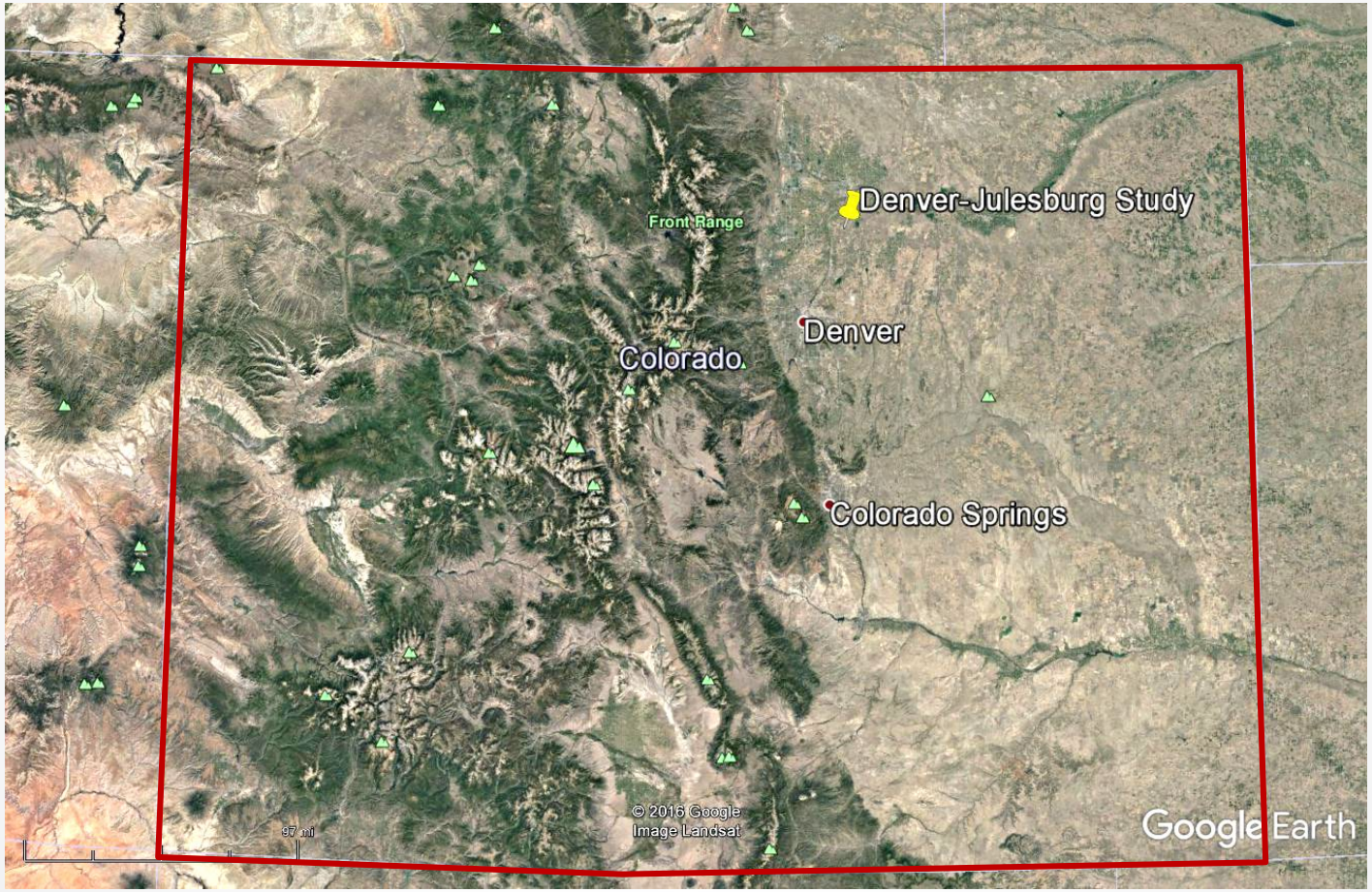
Detroit field study

- Field measurements conducted from Sept. 2010 – June 2011
- Continuous measurements of CO, NO_X, BC, PM_{10}, $PM_{2.5}$, winds, RH
- Monitoring 100 m west of the roadway and at 20, 100, and 300 m east of the roadway.
- On-site traffic monitoring, vehicle counts in each lane

Las Vegas and Detroit study considerations

- Emissions based on vehicle counts and MOVES emissions modeling
  - i.e., greater uncertainty in emissions than studies based on tracer data or on CEMS data
- For NO_2 evaluations, no on-site ozone monitoring
- Up-wind/down-wind configuration allows for clear delineation of background
- Well-characterized dataset, i.e., multiple studies already completed
  - Estimation of on-road NO_2 concentrations, NO_2/NO_X ratios, and related roadway gradients from near-road monitoring data, Richmond-Bryant, et al. Air Qual Atmos Health, 2017, 10: 611. https://doi.org/10.1007/s11869-016-0455-7
  - NO to NO_2 conversion rate analysis and implications for dispersion model chemistry methods using Las Vegas, Nevada near-road field measurements, Kimbrough, et al, Atm. Env, Vol 165, 2017, 23-34, https://doi.org/10.1016/j.atmosenv.2017.06.027

Denver-Julesburg Basin, Colorado Drill Rig NO_2 Monitoring Study

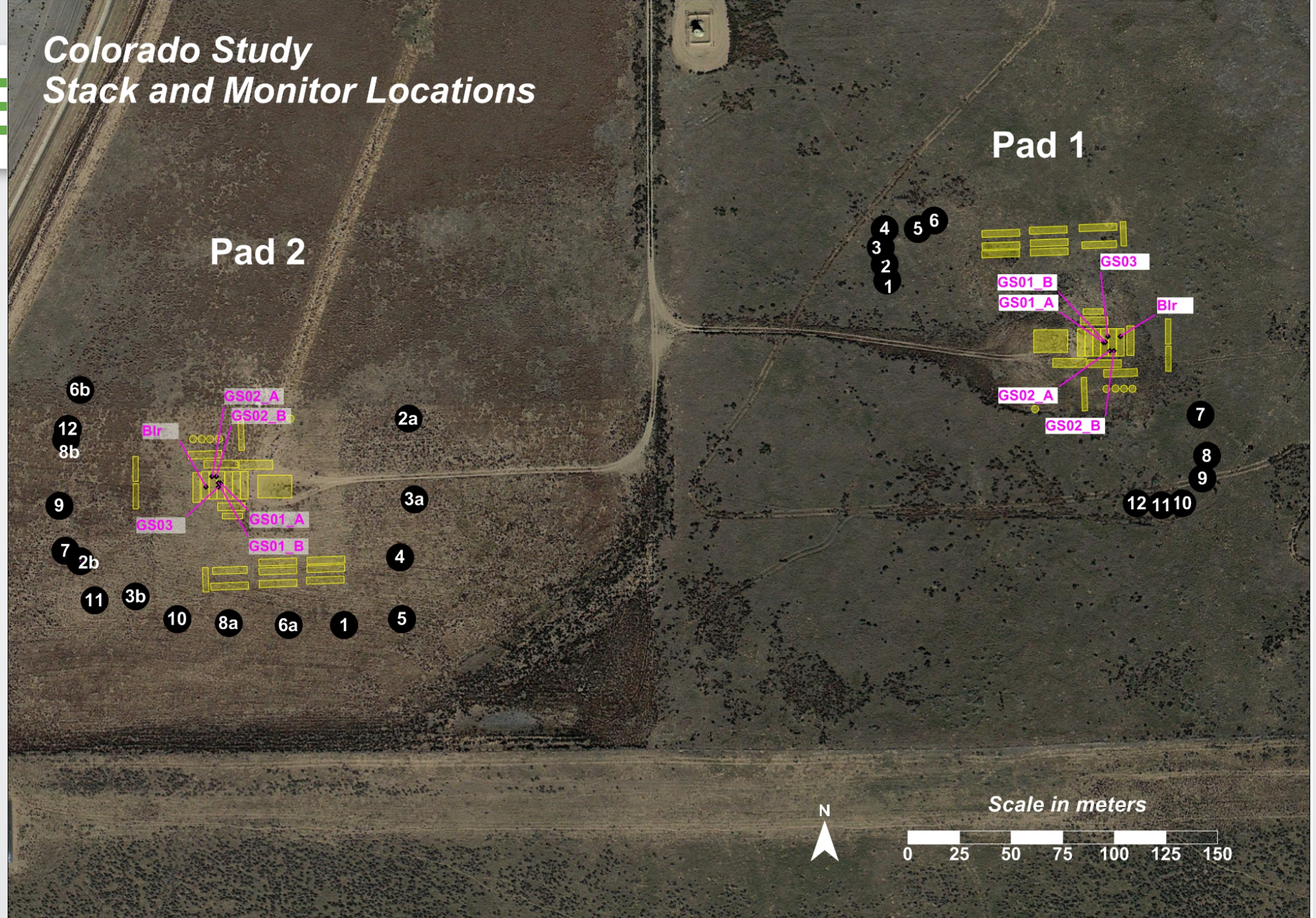


Collaborative Effort

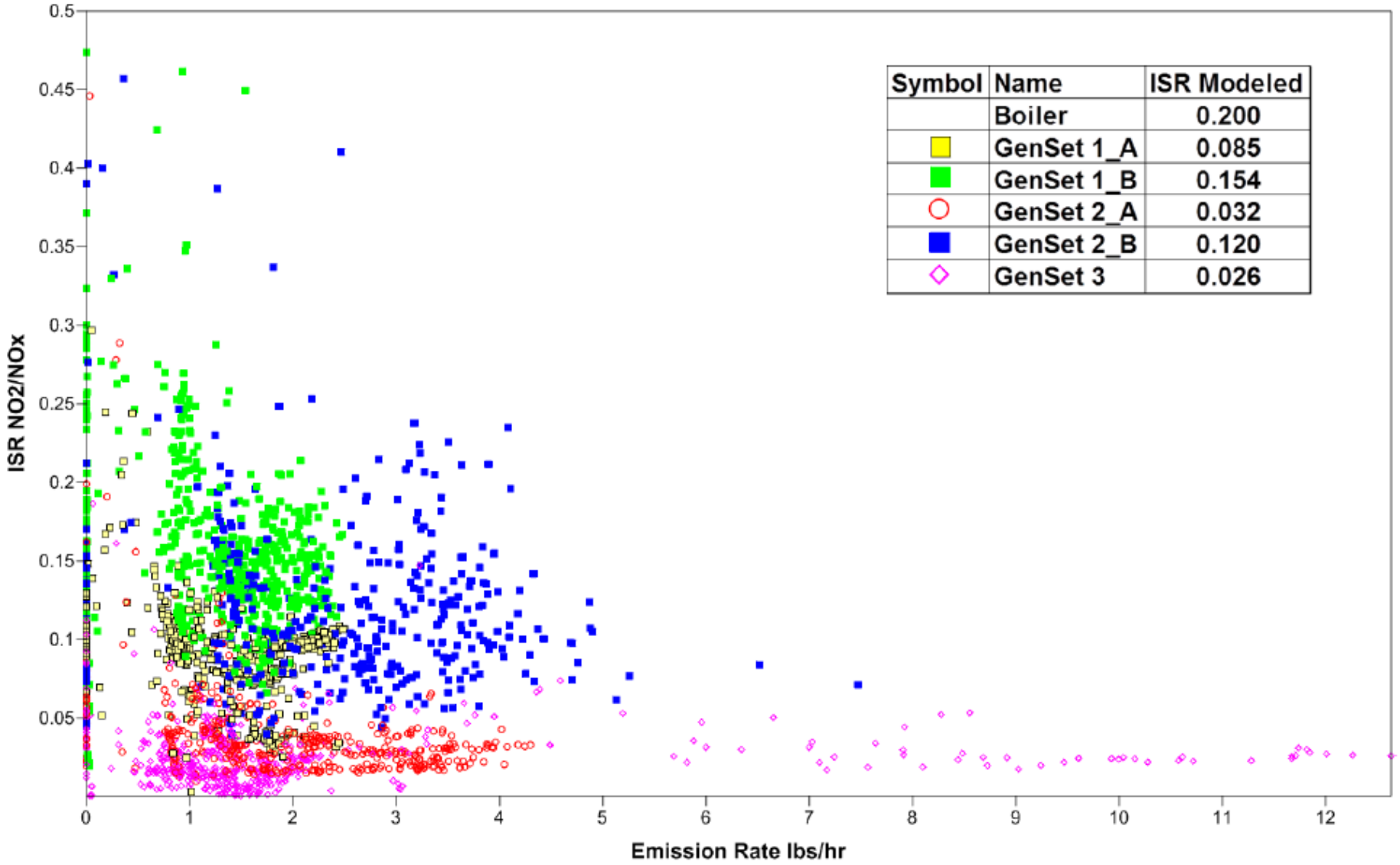
- American Petroleum Institute (API)
- Bureau of Land Management (BLM)
- Anadarko (Colorado)
- ERM
- AECOM
- US EPA

Monitoring Period

- October 10 – November 16, 2014
- Adjacent Well Pads (Pad 1, Pad 2)
- 12 Ambient AQ Monitors
- 3 Discrete Monitoring Configurations for Evaluation
  - Pad 1:October 10, 2014 - October 26, 2014
  - Pad 2a:November 3, 2014 - November 8, 2014
  - Pad 2b:November 10, 2014 - November 16, 2014


Colorado Study
Stack and Monitor Locations
Pad 1
Pad 2
4
5
6
3
2
1
GS03
GS01_B
GS01_A
Blr
GS02_A
GS02_B
7
8
9
12
11
10
6b
12
8b
9
7
2b
11
3b
10
8a
6a
1
5
4
3a
2a
GS02_A
GS02_B
Blr
GS03
GS01_A
GS01_B
N
Scale in meters
0
25
50
75
100
125
150

Hourly in-stack NO_2/NOx Ratios



Current Colorado Workgroup Members

- **ERM - Mark Garrison**
- AECOM – Bob Paine, Chris Warren
- API – Cathe Kalisz
- US EPA OAQPS – Chris Owen, Clint Tillerson
- US EPA Region 1 – Leiran Biton
- US EPA Region 7 – Lance Avey
- **US EPA Region 8 – Rebecca Matichuk**
- City of Denver – Mohamed Eltarkawe, Michael Ogletree, Gregg Thomas
- Westar – Tom Moore, Doug Blewitt, Nicole Downey
- BLM – Erik Vernon, Forrest Cook

OK Compressor Station Field Study

- PRCI CPS-11-5: Ambient NO_2 Modeling for 1 Hour Standard
- Four monitor locations
  - 3 “impact” and 1 “background”
- Meteorology – 2, 10, and 30 meter
- Emissions data from engines using PEMS
- Monitoring commenced Dec 1, 2015 and completed Dec, 2016