

Evaluation of AERMOD with an Alternate NO_x Chemistry Scheme

EPA 11th Conference on Air Quality Modeling
August 12-13, 2015
Research Triangle Park, NC



Cathe Kalisz
kaliszc@api.org

AERMOD with Alternate NO_x Chemistry

BACKGROUND:

- The Atmospheric Dispersion Modeling System (ADMS) is widely used internationally.
- A 2013 modeling study done by an API member company suggested that the ADMS NO_x chemistry module may have better predictive skill than the NO₂ options currently available in AERMOD (version 14134).
- The following slides compare performance of AERMOD coded with an ADMS chemistry option to current AERMOD Tier 3 NO₂ options.
- We will be updating these evaluations using the proposed version of AERMOD and proposed NO₂ options, including PVMRM2.

AERMOD with ADMS NO_x Chemistry

ADMS Chemistry Module:

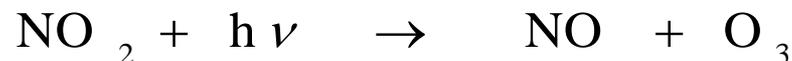
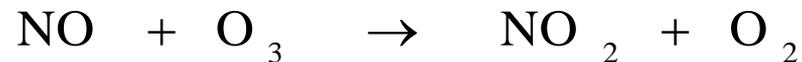
The work to date incorporates the “standard” ADMS chemistry module

Inputs

- Emission rates of NO_x and NO₂
- Hourly background values for NO_x, NO₂ and O₃

Methodology

- NO_x and NO₂ concentrations calculated at each receptor
- At each receptor calculate the weighted (by source contribution) mean travel time of pollutant
- Add background concentrations
- Apply chemical reactions over mean travel time of pollutant



AERMOD with ADMS NO_x Chemistry

- ❑ **Two key differences between ADMS Chemistry Module and AERMOD Tier 3 NO₂ Options:**
 - ⇒ ADMS module includes reactions for both NO ozone titration and NO₂ photolysis.
 - ⇒ ADMS module accounts for chemical reaction rate.

- ❑ **For work done using AERMOD version 14134, no significant difference in model run time between ADMS chemistry module and Tier 3 options.**

Differences between AERMOD & ADMS Chemistry schemes

Model	ADMS		AERMOD			
Chemistry scheme	Standard ADMS	Dilution & Entrainment	ARM2	OLM	PVMRM	Standard ADMS in AERMOD
NO _x ratio scheme			Empirical scheme			
Ozone conversion scheme	Yes	Yes		Yes	Yes	Yes
Full reaction scheme including photolysis	Yes	Yes				Yes
Entrainment of background ozone into plume	Full	Yes		Yes		Yes
	Consistent with plume dilution		Yes		Yes	

Results for **OLM**, **PVMRM** and the **Standard ADMS chemistry scheme implemented within AERMOD 14134** are shown on the following slides

AERMOD with ADMS NO_x Chemistry

Preliminary Results for 5 Datasets

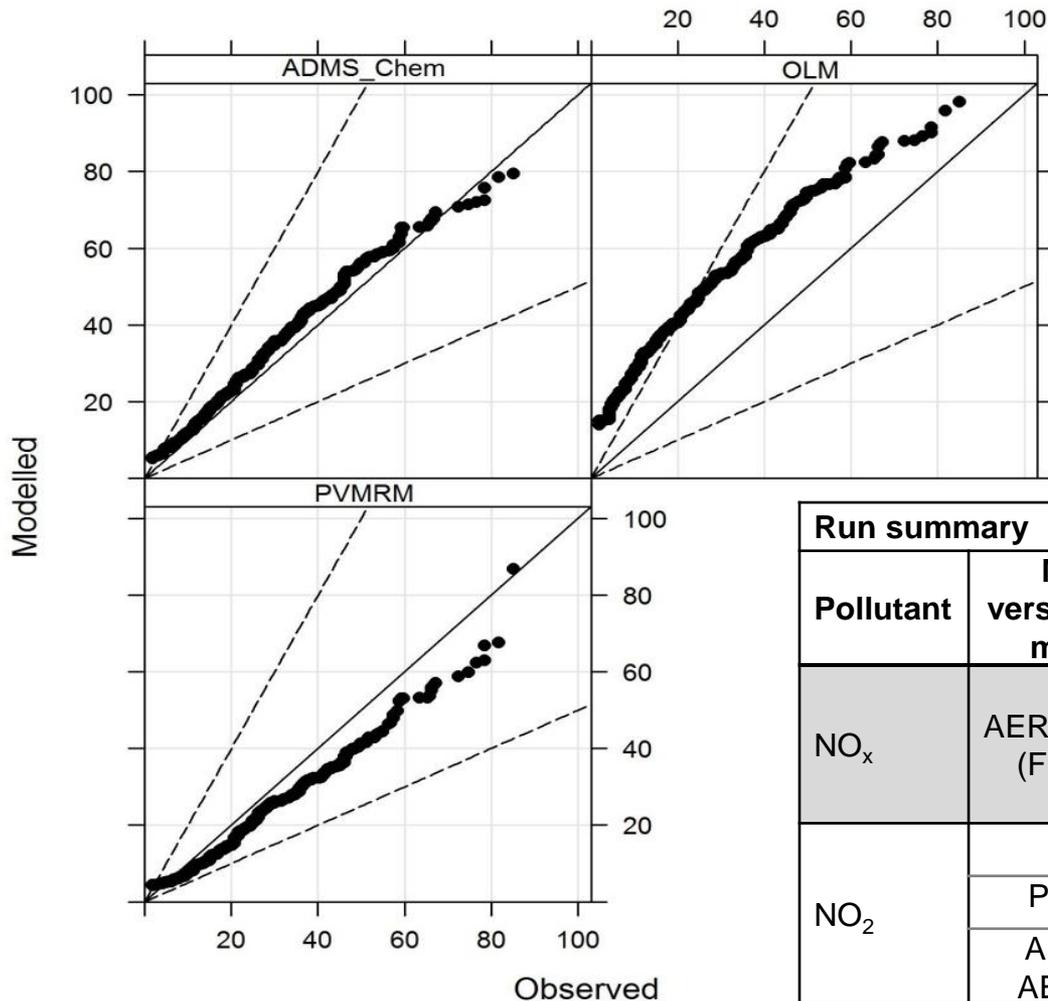
Study	Approximate source to receptor distance (m)	Downstream distance regime
Palaau	~ 220	Near field
Empire Abo (North)	1600	Far field
Empire Abo (South)	2500	Far field
Wainwright	500	Mid field
Prudhoe Bay	60	Near field

Dataset adjustments:

NO₂/NO_x in-stack ratios for Palaau and Empire Abo sources changed from 20% to 10%

Comparison for Palaau Dataset

Quantile - Quantile Plots - NO₂ (µg/m³)



Correlation between Observed and Modeled NO₂/NO_x ratios

OLM 0.40

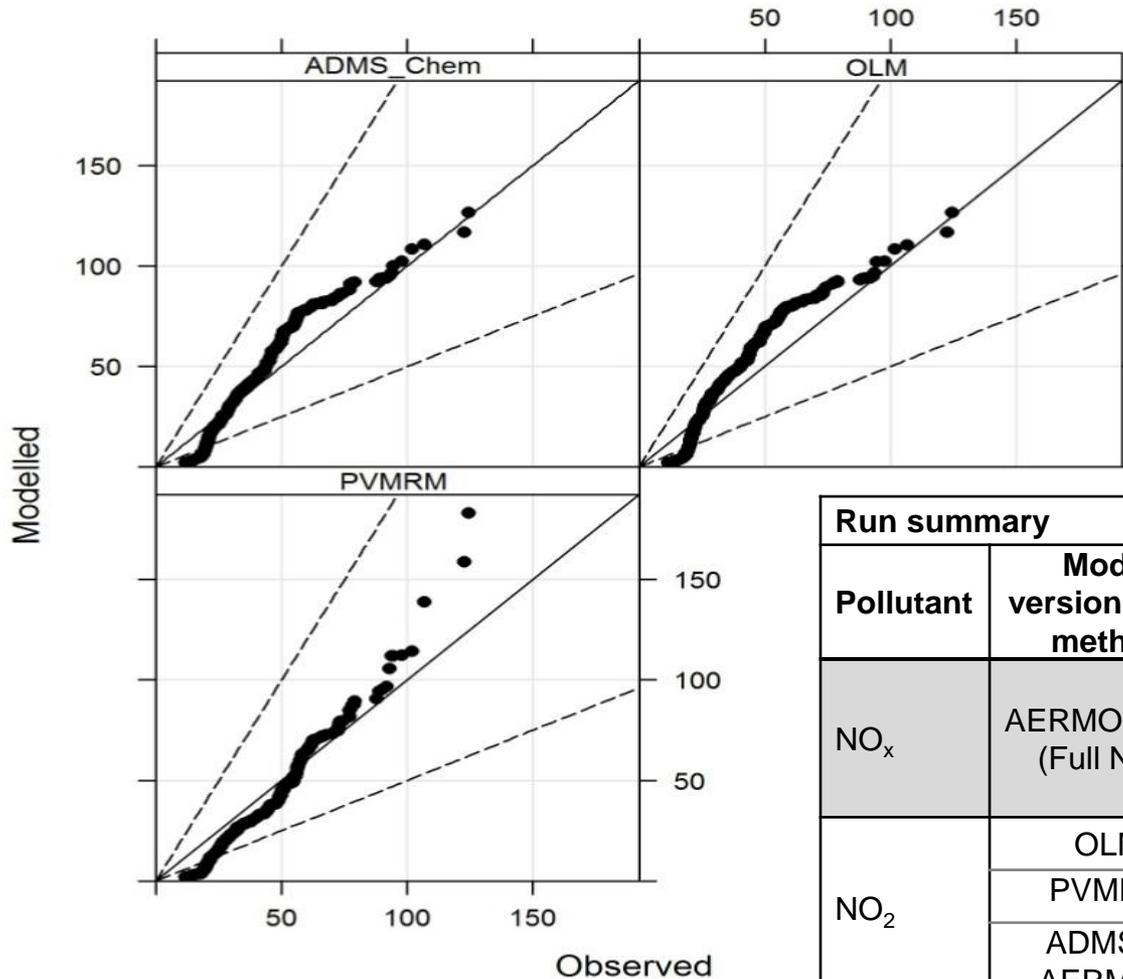
PVMRM 0.71

ADMS_Chem 0.70

Run summary		Statistical summary (µg/m ³)			
Pollutant	Model version / NO ₂ method	Obs Max	Mod Max	Obs RHC	Mod RHC
NO _x	AERMOD NO _x (Full NO ₂)	642	459	659	493
NO ₂	OLM	85	98	95	105
	PVMRM	85	87	95	87
	ADMS in AERMOD	85	79	95	88

Comparison for Empire Abo North Dataset

Quantile - Quantile Plots - NO₂ (µg/m³)



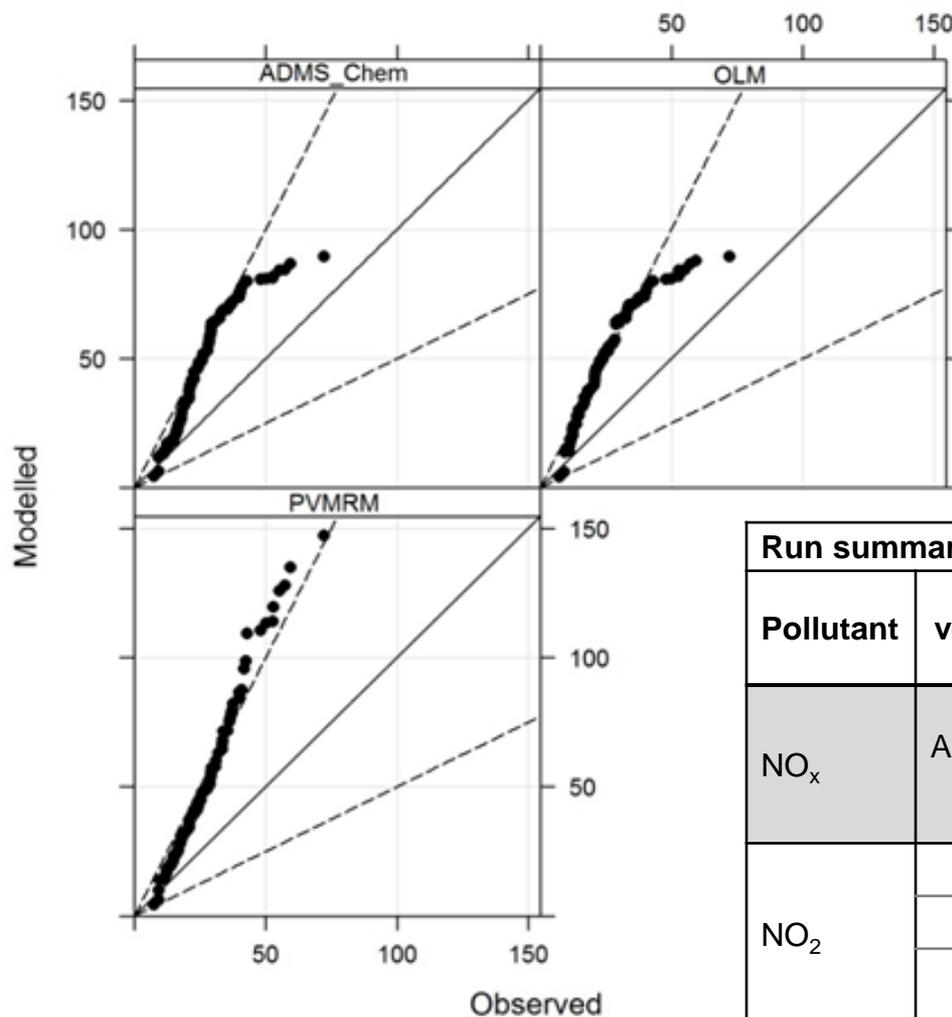
Correlation between Observed and Modeled NO₂/NO_x ratios

OLM	0.17
PVMRM	0.06
ADMS_Chem	0.25

Run summary		Statistical summary (µg/m ³)			
Pollutant	Model version / NO ₂ method	Obs Max	Mod Max	Obs RHC	Mod RHC
NO _x	AERMOD NO _x (Full NO ₂)	561.0	449.8	534.6	479.6
NO ₂	OLM	124.6	126.5	129.7	124.6
	PVMRM	124.6	183.1	129.7	164.5
	ADMS in AERMOD	124.6	126.6	129.7	124.5

Comparison for Empire Abo South Dataset

Quantile - Quantile Plots - NO₂ (µg/m³)



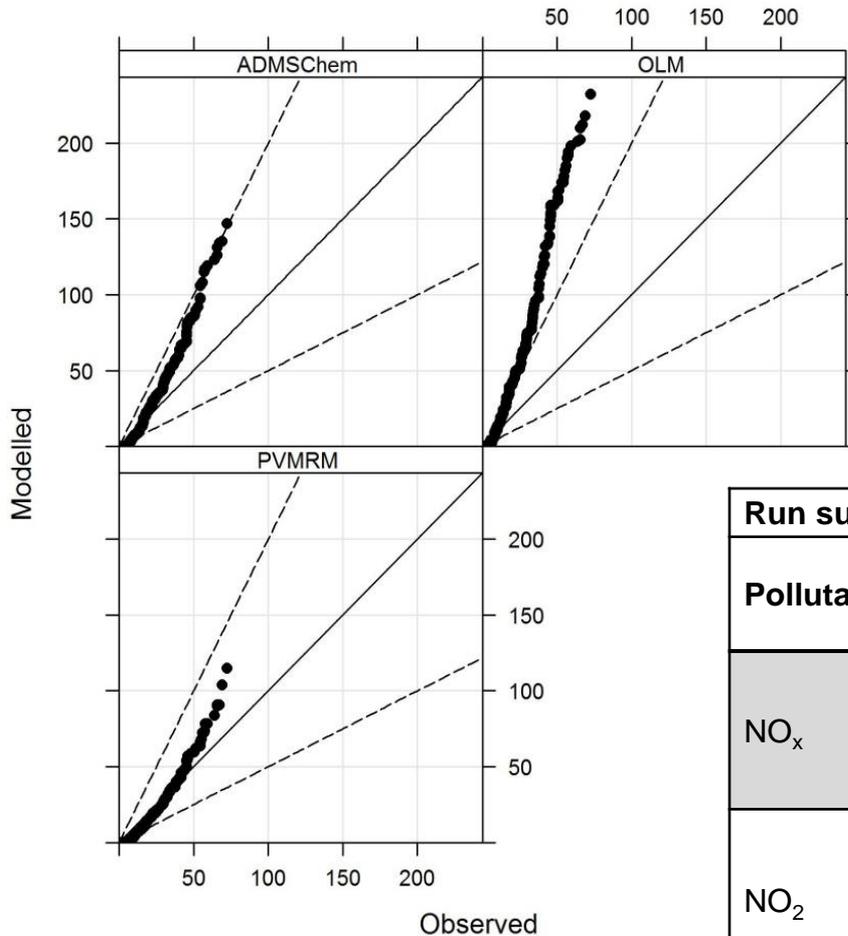
Correlation between Observed and Modeled NO₂/NO_x ratios

OLM	0.04
PVMRM	- 0.24
ADMS_Chem	0.19

Run summary		Statistical summary (µg/m ³)			
Pollutant	Model version / NO ₂ method	Obs Max	Mod Max	Obs RHC	Mod RHC
NO _x	AERMOD NO _x (Full NO ₂)	388.1	283.8	417.1	358.3
NO ₂	OLM	72.2	89.5	71.2	97.6
	PVMRM	72.2	147.2	71.2	173.5
	ADMS in AERMOD	72.2	89.6	71.2	97.9

Comparison for Wainwright Dataset

Quantile - Quantile Plots - NO₂ (µg/m³)



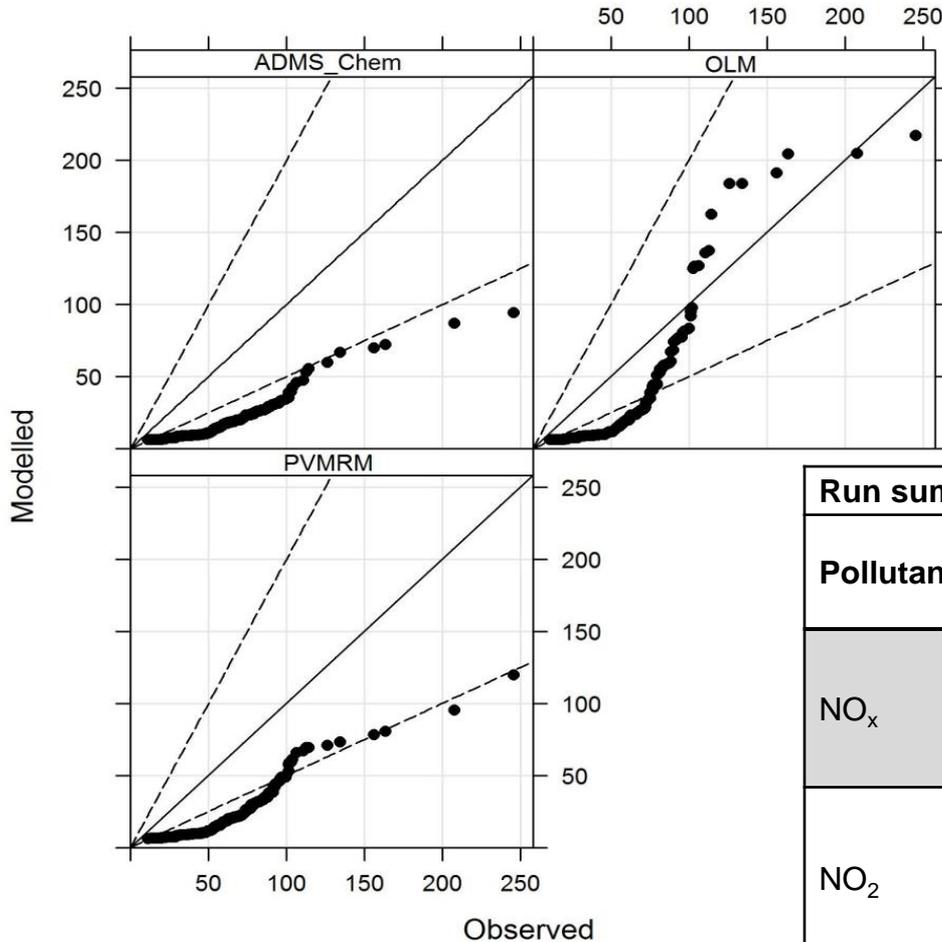
Correlation between Observed and Modeled NO₂/NO_x ratios

OLM	0.02
PVMRM	- 0.07
ADMS_Chem	0.36

Run summary		Statistical summary (µg/m ³)			
Pollutant	Model version / NO ₂ method	Obs Max	Mod Max	Obs RHC	Mod RHC
NO _x	AERMOD NO _x (Full NO ₂)	369	609	412	730
NO ₂	OLM	72	232	83	264
	PVMRM	72	115	83	119
	ADMS in AERMOD	72	147	83	175

Comparison for Prudhoe Bay Dataset

Quantile - Quantile Plots - NO₂ (µg/m³)



Correlation between Observed and Modeled NO₂/NO_x ratios

OLM - 0.11

PVMRM - 0.05

ADMS_Chem 0.25

Run summary		Statistical summary (µg/m ³)			
Pollutant	Model version / NO ₂ method	Obs Max	Mod Max	Obs RHC	Mod RHC
NO _x	AERMOD NO _x (Full NO ₂)	845	307	759	333
NO ₂	OLM	246	217	190	251
	PVMRM	246	120	190	123
	ADMS in AERMOD	246	94	190	91

Summary of NO₂ Comparisons

❑ OLM

- Generally over predicts the NO₂ concentration
- Has the lowest proportion of values within a factor of two of the observed
- NO₂/NO_x ratio correlations are generally poor

❑ PVMRM

- Demonstrates the best mean NO₂ concentration
- Has a reasonably high proportion of values within a factor of two of the observed
- NO₂/NO_x ratio correlations are generally poor; modelled and observed values negatively correlated for three of the five datasets considered

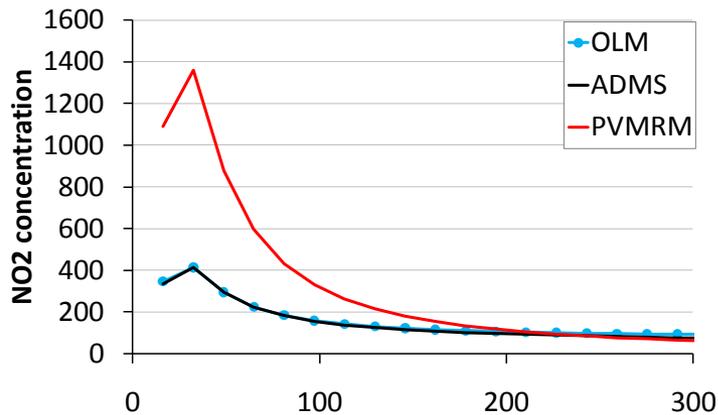
❑ ADMS chemistry module

- Generally over predicts the NO₂ concentration
- Has a reasonably high proportion of values within a factor of two of observed concentrations
- Shows the most consistent performance considering the correlation for the NO₂/NO_x ratio

Example - Sensitivity Modeling

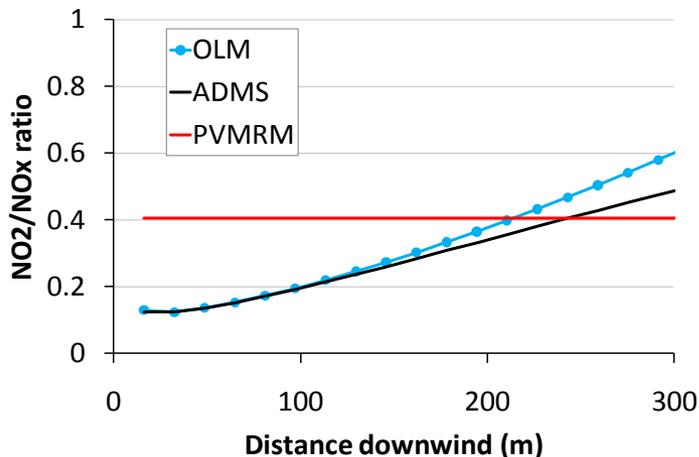
Sensitivity tests comparing the 3 modules were done for a single, non-buoyant source (12.5 m stack height) under various meteorological conditions.

Example *near-field* NO_2 concentrations for *stable early morning, moderate wind speed conditions*:



PVMRM higher than OLM upper bound for conversion of NO to NO₂

The inputs for this near-field scenario were used in AERMOD v15181; PVMRM2 predictions similar to those for PVMRM in AERMOD v14134.



AERMOD with Alternate Chemistry Scheme – Next Steps

- Add the ADMS chemistry code to the proposed version of AERMOD (v15181) and rerun the evaluations.
- Conduct additional sensitivity testing using single and multi-source scenarios.
- Conduct additional evaluations using WRAP NO₂ datasets for Colorado and Alaska.
- Make further modifications to the standard ADMS chemistry module to use a simplified version of the ADMS dilution and entrainment scheme in AERMOD, drawing on some of the parameters used by PVMRM2.

As we move forward, it will be important to have a regulatory process that provides for timely testing and incorporation of model improvements.