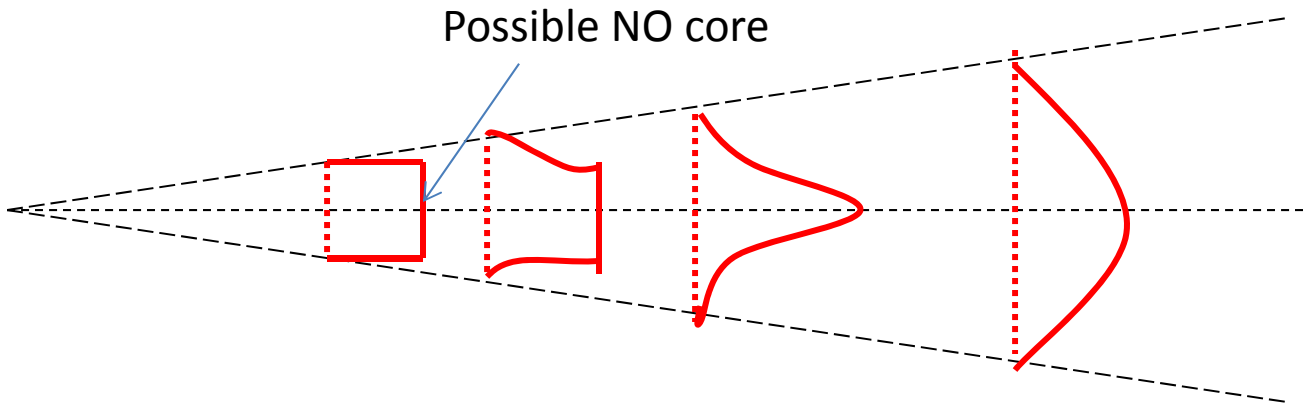
Issues Associated With NO_2 Model Evaluation

Doug Blewitt, CCM
AQRM
Nicole Downey, Ph.D.
Earth System Sciences, LLC

Conceptual NO/NO_2 Plume Model



Attributes:

1) Reaction of $NO + O_3 = NO_2$ is a quasi instantaneous reaction in a well mixed system
2) The rate of reaction is controlled by:
   - Entrainment of ambient air containing O_3 into the plume
   - Ozone concentration
   - Rate of reaction
3) Because the rate of entrainment occurs at the edges of the plume, the conversion of NO into NO_2 can be very retarded and the complete conversion into NO_2 can be at substantial downwind distances (NO plume core)
4) **AERMOD assumes that $[NO_2] = [NOx] * [NO_2]/[NOx]$**
5) **Model must predict total dispersion (NOx) as well as the fraction of NO_2**
6) **NO2 model performance cannot be better than for NOx unless there are compensating errors**

Empire Abo NO_2 Model Performance Database

- One of the primary datasets used to evaluate 1 hr NO_2 model performance by Aermod
- Empire Abo - Amoco Production (BP) Gas Plant
- Data was collected in 1993/1994
- Monitoring program was designed to develop a database for performing OLM calculations to demonstrate compliance with NMED 24-hour NO_2 standard
- Monitoring network designed so that one ozone monitor was always upwind of the plant – quantify O_3 scavenging by NO_2
- Empire Abo plant is not an isolated source therefore regional impacts should be analyzed

Limitations to Empire Abo Database

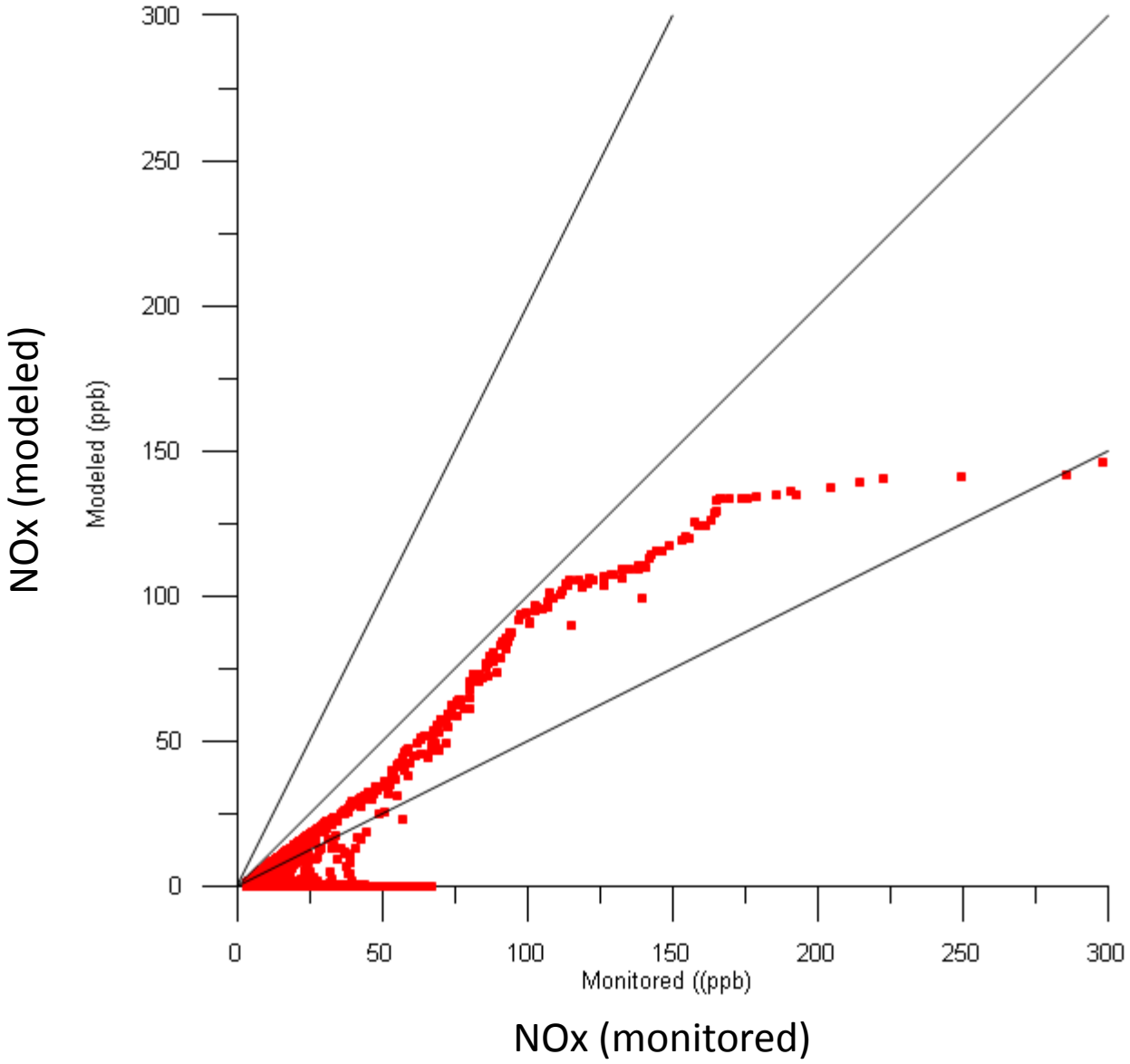
- There are at least 3 different emission inventories associated with the facility and all represent permitted capacity
  - Most likely case – 2,600 t/yr based on historical plant operating capacity
  - Compliance inventory – 1,852 t/yr
  - 1995 inventory based on 24-hour NMED compliance strategy – 1,549 t/yr probably performed after monitoring was completed (EPA likely using this inventory)
- In addition, compressor engines did not have air fuel ratio controllers and hence emissions may have drifted from optimal levels
- **Conclusion - Facility emissions are not well known and use of the Empire Abo database for NO2 model performance is very speculative**
- Questions regarding how EPA used the database

Other NO_2 Databases

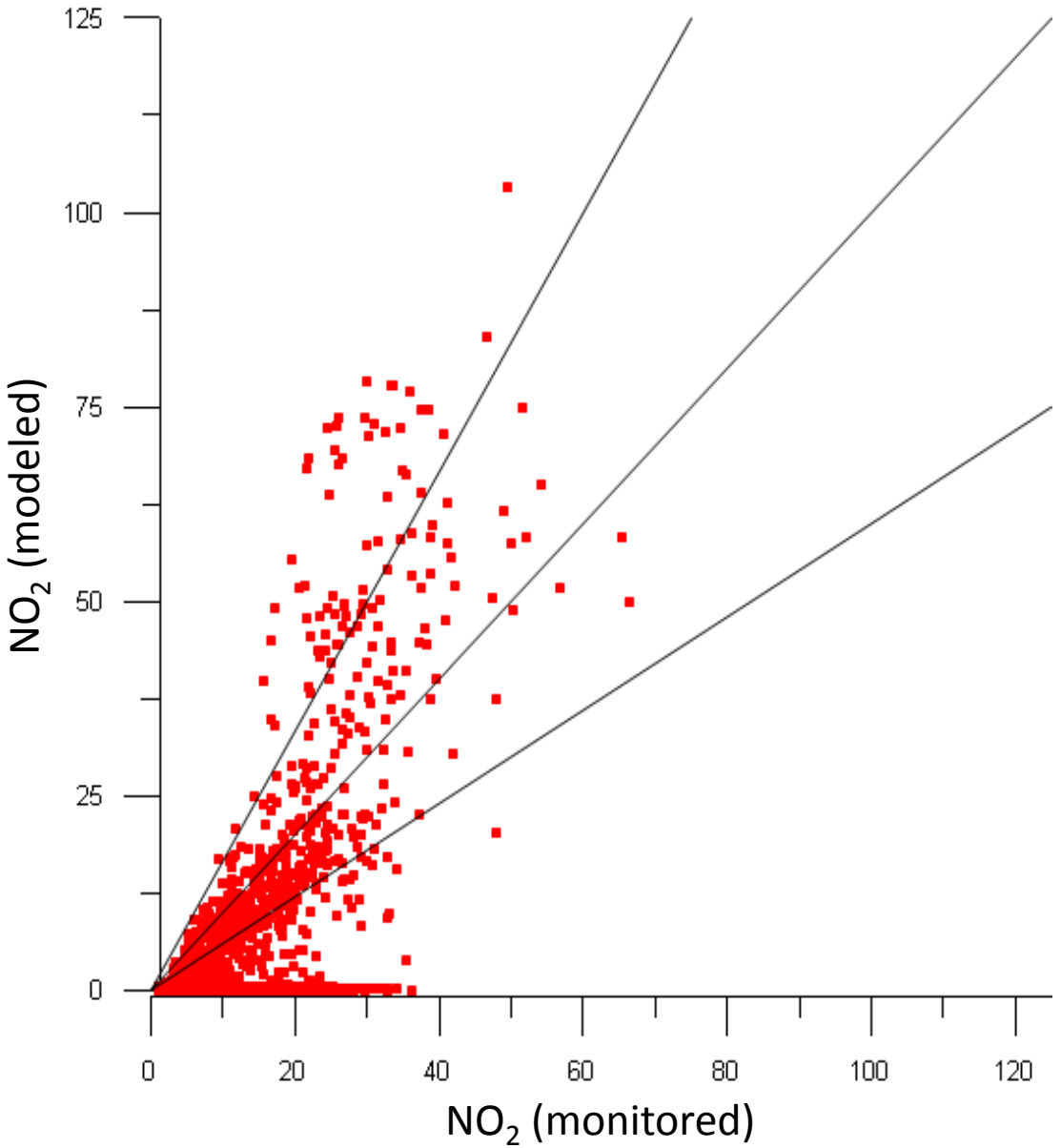
- Palaau, HI – Oil fired turbine and very little is know regarding that database
- Wainwrite, AK – Oil fired electric generators – Very low O_3, NO_x and NO_2 concentrations
- EPA needs to conduct a comprehensive NO_2 field program for NO_2 model evaluation

NO_2 Model Performance

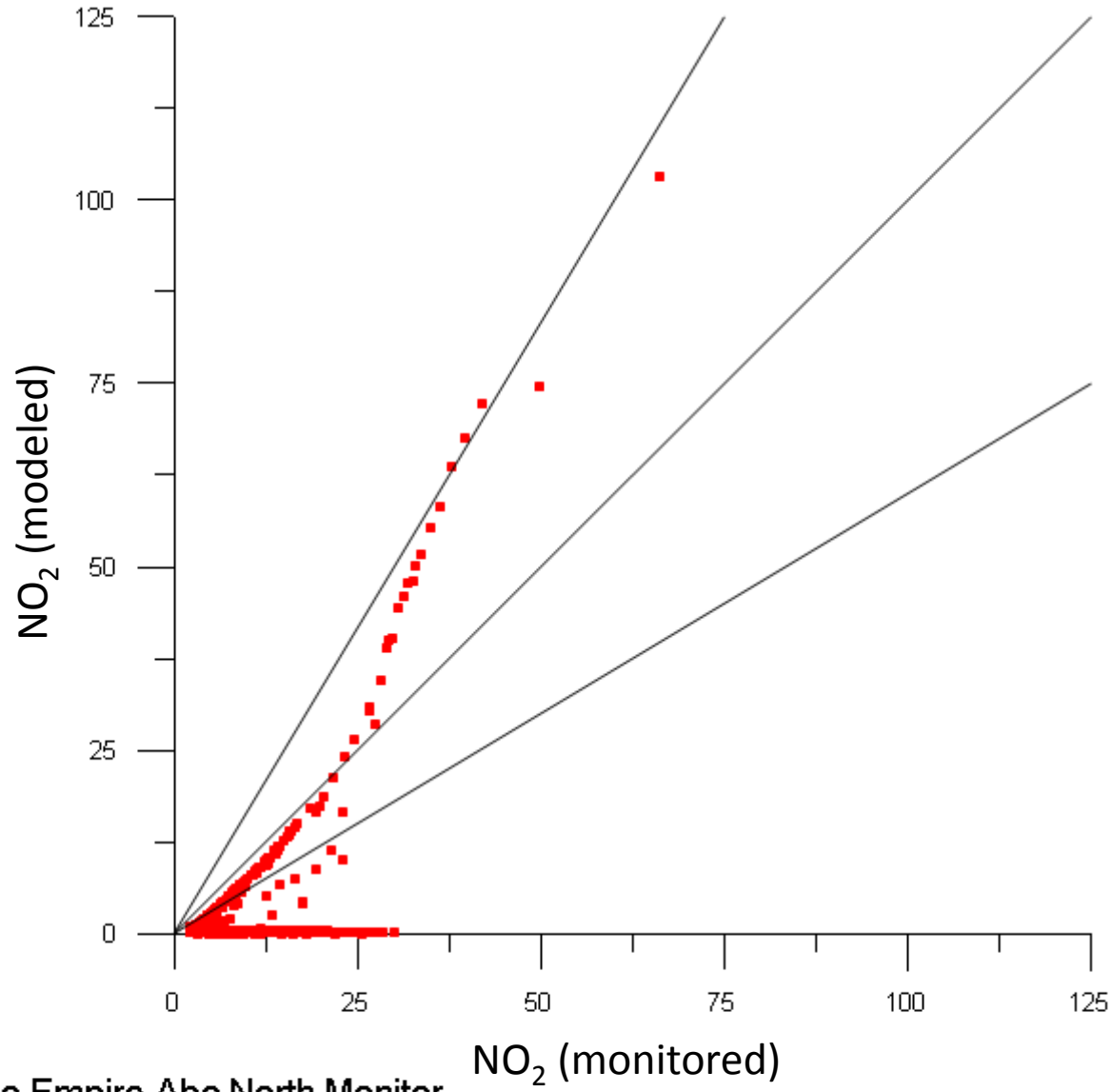
- NO_2 model accuracy evaluation must compare model predictions to observations in three different ways
  - NOx model predictions compared to NOx observations (unpaired in time) – Evaluates total dispersion
  - NO_2 model predictions compared to NO_2 observations (using NOx pairing) – Evaluates total dispersion and NO2 chemistry matching dispersion and chemistry
  - NO_2 model predictions compared to NOx observations (unpaired in time) -> current EPA approach



NOx Empire Abo North Monitor
Unpaired in time
Sort based on NOx
1995 emission inventory used (EPA used this inventory)



NO2 Empire Abo North Monitor
Unpaired in Time
Sort based on NOx
1995 Emission Inventory Used (EPA used this inventroy)
Ozone data based on South Site

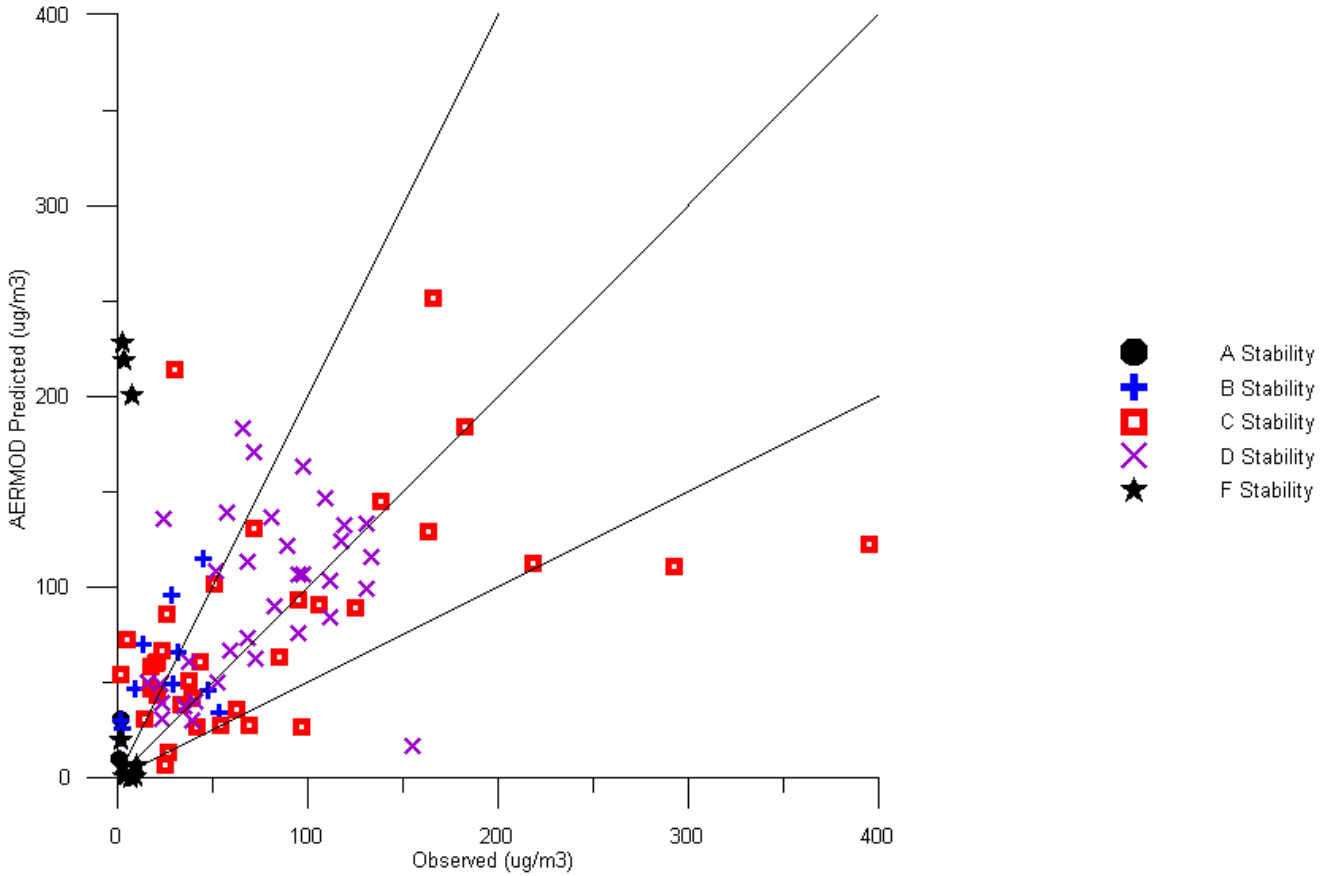


NO2 Empire Abo North Monitor
Unpaired in Time
Sort based on NO2
1995 Emission Inventory Used (EPA used this inventroy)
Ozone data based on South Site

Conclusions Regarding NO_2 Model Performance for Empire Abo

- In spite of the uncertainties in emission data, NO_x model performance is underestimated by almost a factor of two
- If NO_2 is evaluated using NO_x pairing, NO_2 model performance is over stated by more than a factor of two – implies that matching NO_2 conversion with NO_x dispersion overstates NO_2 formation (compensating errors)
- If NO_2 is compared to monitoring data independent of time, NO_2 over predicts by a factor of two (compensating errors)
- EPA's analysis should be publicly available and described (i.e. what emission inventory was used, which ozone monitor, etc…)

Why Is the Identification of Compensating Errors Important?



AERMOD Model Performance for AGA Data Base

Conclusions and Recommendations

- Code review of AERMOD PVMRM has formulation problems (Hanna presentation)
- Conversion of NO into NO_2 overstates NO_2 conversion (Empire Abo analysis)
- There is an urgent need for EPA to develop refined NO_2 modeling procedures and databases for evaluation
- Until refined techniques occur, EPA should adopt ARM2