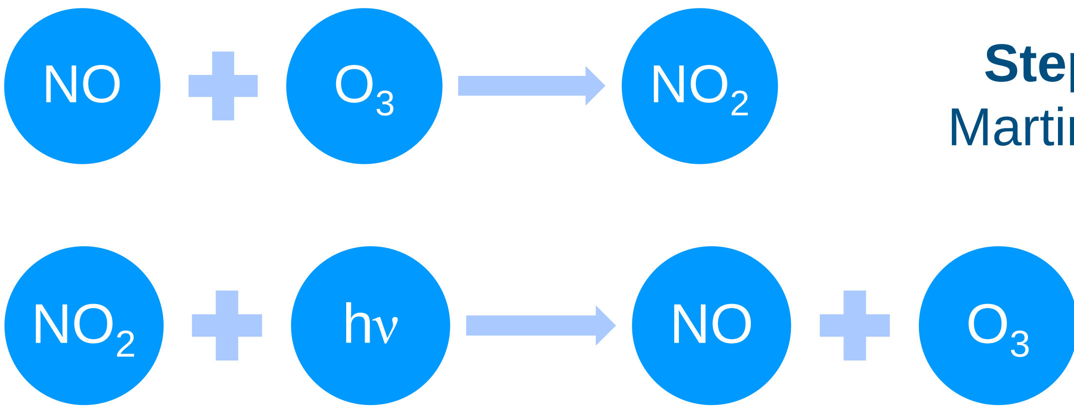
A validation study of the ADMS plume chemistry schemes



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Where does NO_2 come from?

- Downwind of an industrial source, NO_2 arises from three main contributions:

Long-range transport & long timescale chemistry

- Ambient background level of NO_2 in the atmosphere.
- Long-range transport of emissions and long timescale chemical reactions.

Primary emissions of NO_2

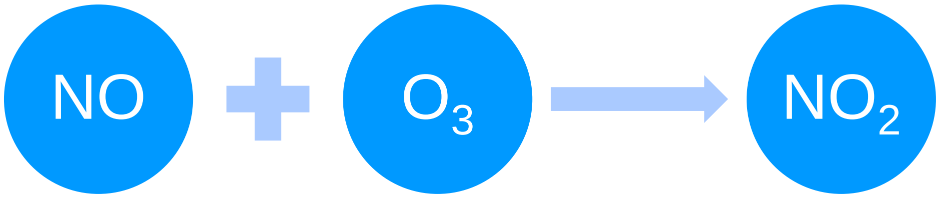
- A proportion of NO_x is emitted as NO_2.
- Proportion depends on source type, typically between 5% and 25% for industrial sources.

Secondary NO_2 from short timescale chemical reactions

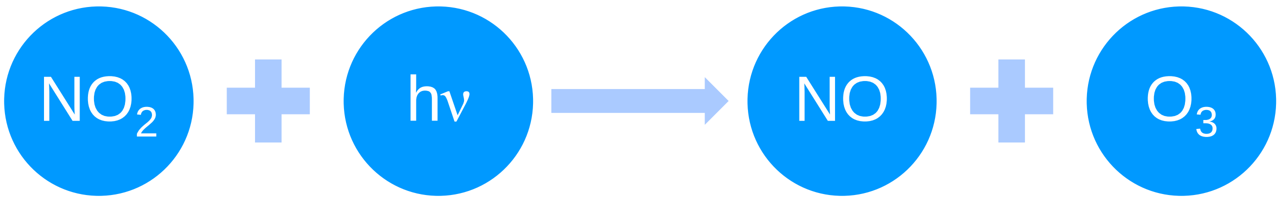
- Away from local sources of NO_x, the background proportion of NO_2 is typically 70% - 95%.
- Secondary NO_2 comes primarily from the oxidation of NO.

NO_x chemistry reactions

- Two short timescale chemical reactions are considered
  - The creation of NO_2:



  - The photolysis of NO_2 by sunlight:

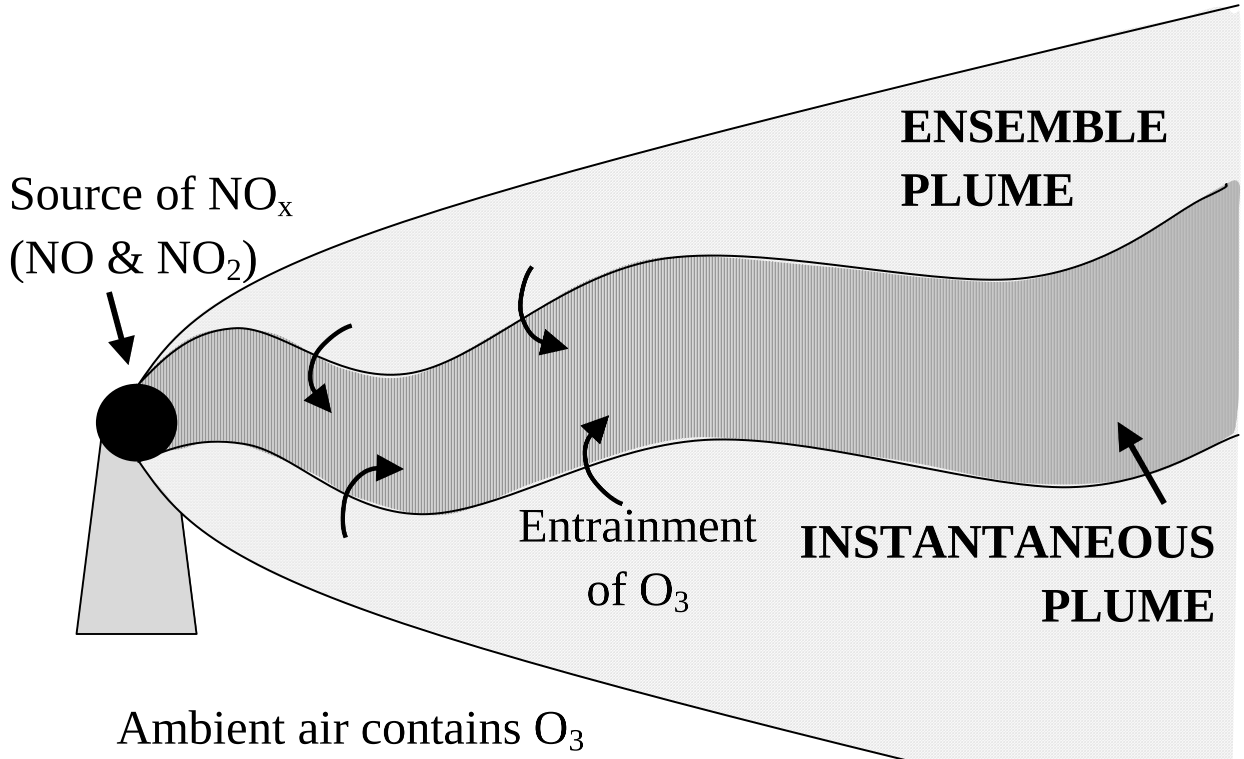


- O_3 comes from atmospheric background – not emitted from sources
- Other chemical reactions occur, but over longer timescales and with species less abundant in an industrial setting.

Modelling a plume

Industrial NO_x source

e.g. generator, power plant, boiler, etc.



NO_x chemistry modelling schemes

Ensemble plume chemistry

- Assumes O_3 well mixed along whole plume
- Chemistry occurs in ensemble plume
- Conservative prediction of NO_2

Instantaneous plume chemistry

- Accounts for amount of background O_3, NO_x and NO_2 entrained into plume
- Chemistry occurs in instantaneous plume
- More theoretically accurate prediction of NO_2

Considerations when validating NO_x chemistry

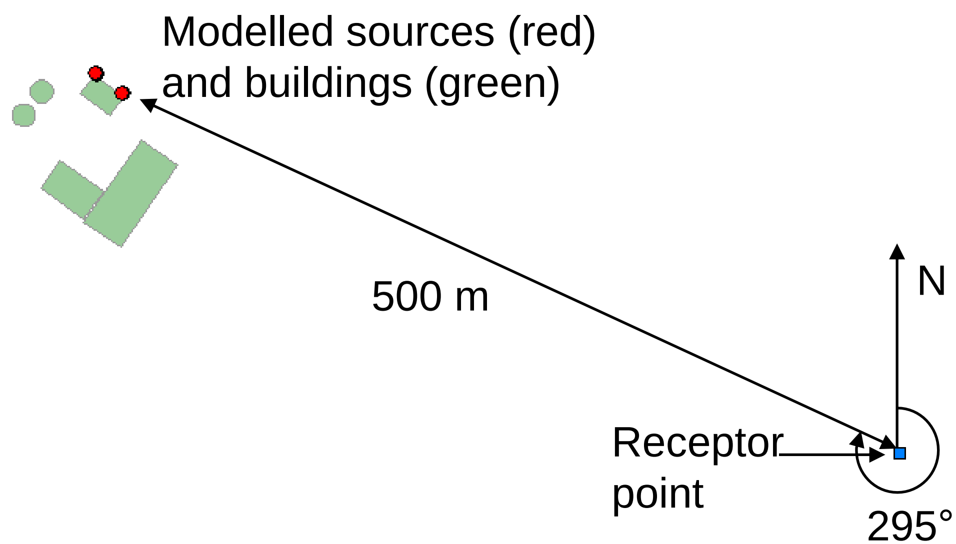
- Two aspects should be considered for NO_2 validation:
  - Dispersion processes – accuracy of NO_x
  - Chemistry processes – accuracy of NO_2
- Not possible to determine NO_2 accuracy independently of NO_x accuracy
- NO_2 performance must be considered in relation to NO_x validation
  - Ideally NO_2 performance would be similar to NO_x performance
  - Cannot expect NO_2 performance to be good if NO_x performance is poor

Note

- Restrict comparisons to appropriate wind directions and hours, when source plume impacts monitors

Case study: Wainwright

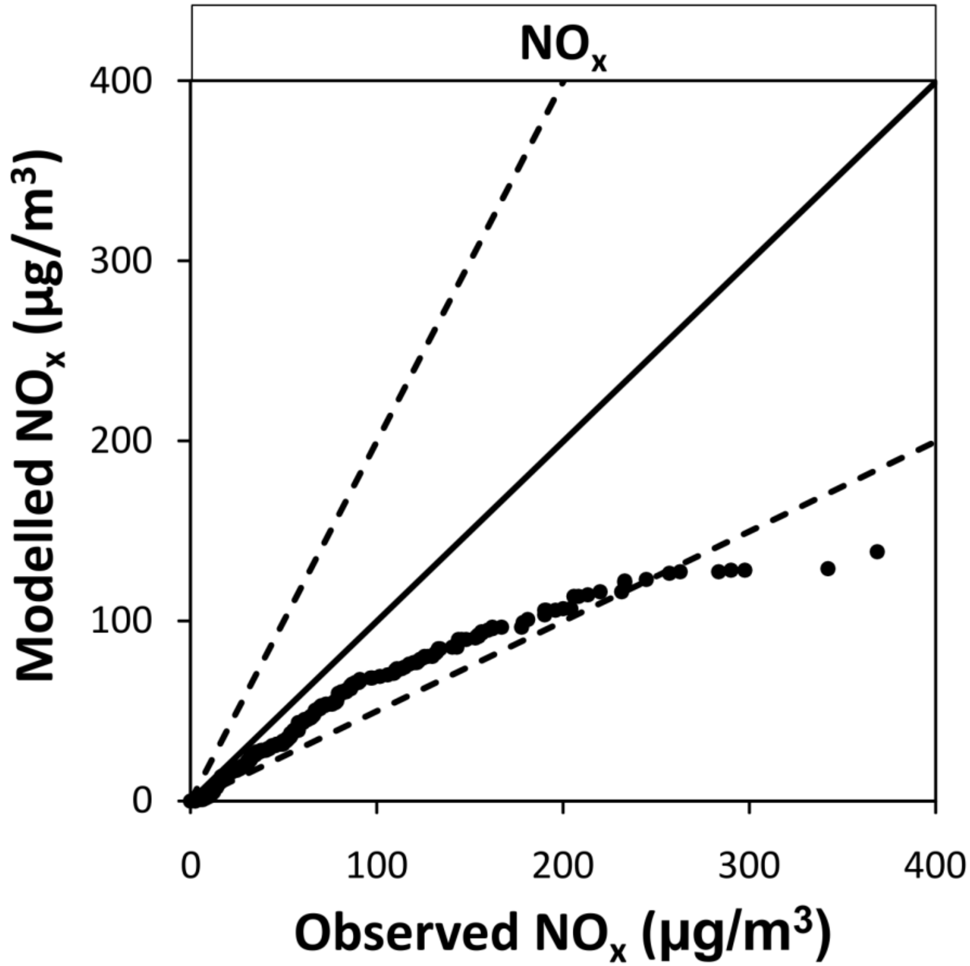
- Validation of ADMS 5 NO_x chemistry with Wainwright dataset:
  - Small, diesel powered power plant in Alaska
  - 5 short stacks, similar to building height, mostly single stack operation
  - Measurement campaign over 12 ½ months
  - Single receptor point



Validation

Case study: Wainwright

NO_x results (μg/m³)

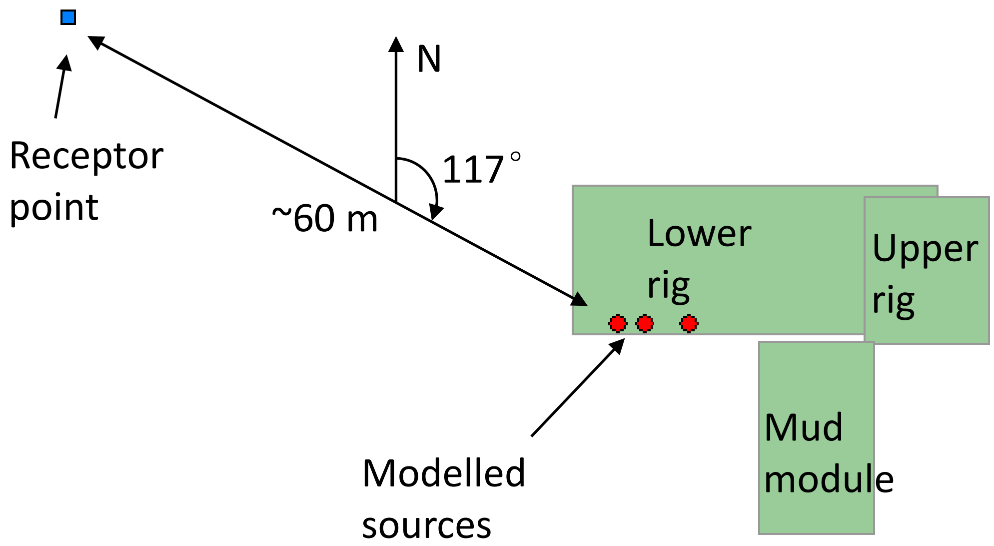


Observed Mean	43
Modelled Mean	26
R	0.79
Fac2	0.52
Observed Max	370
Modelled Max	140

Validation

Case study: Prudhoe Bay

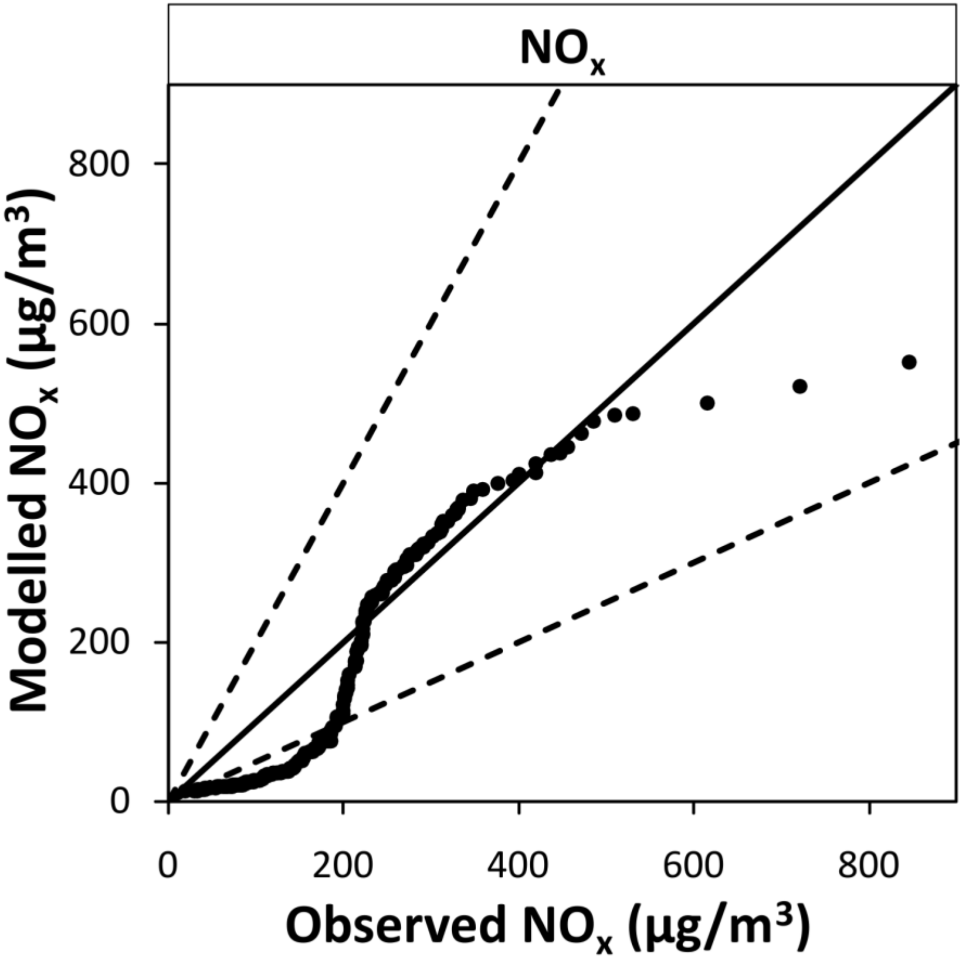
- Oil drilling rig on the North Slope of Alaska
- Measurement campaign over 40 days
- Three largest sources modelled
- One monitor, very close to sources
- Measured NO_x, NO_2 and O_3 concentrations
- Measured met conditions



Validation

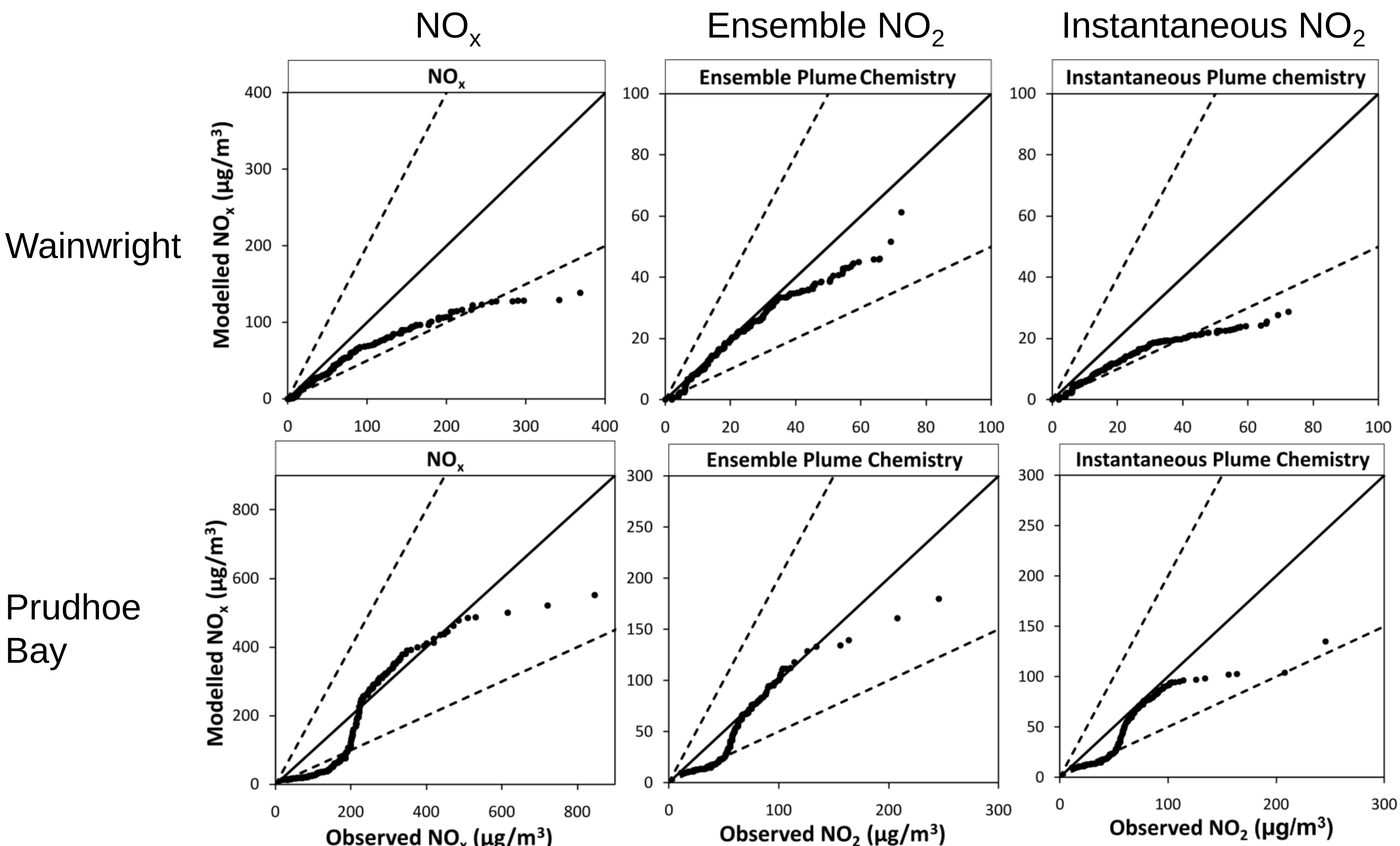
Case study: Prudhoe Bay

NO_x results ($\mu g/m^3$)



Observed Mean	190
Modelled Mean	160
R	0.68
Fac2	0.56
Observed Max	850
Modelled Max	550

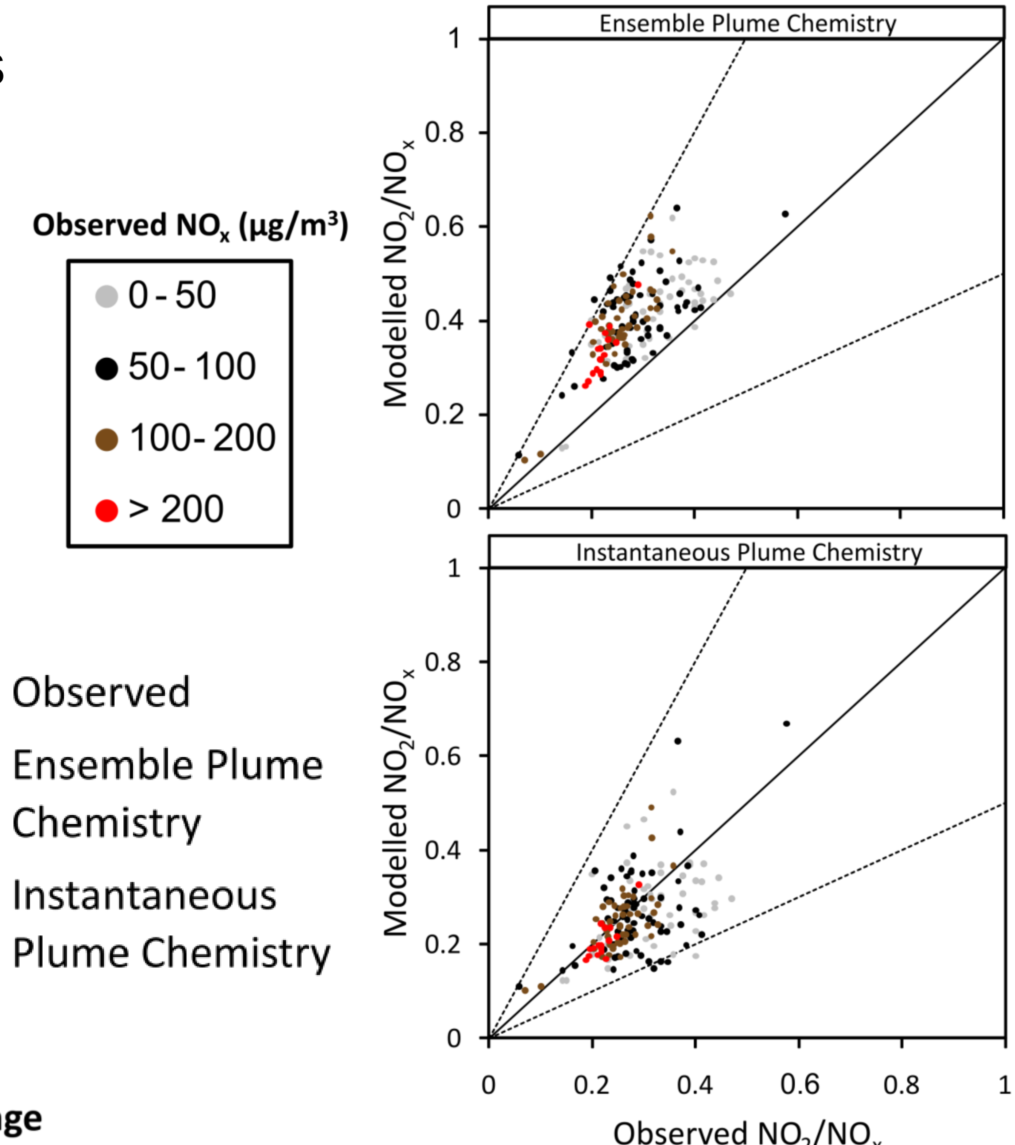
Case studies: Results

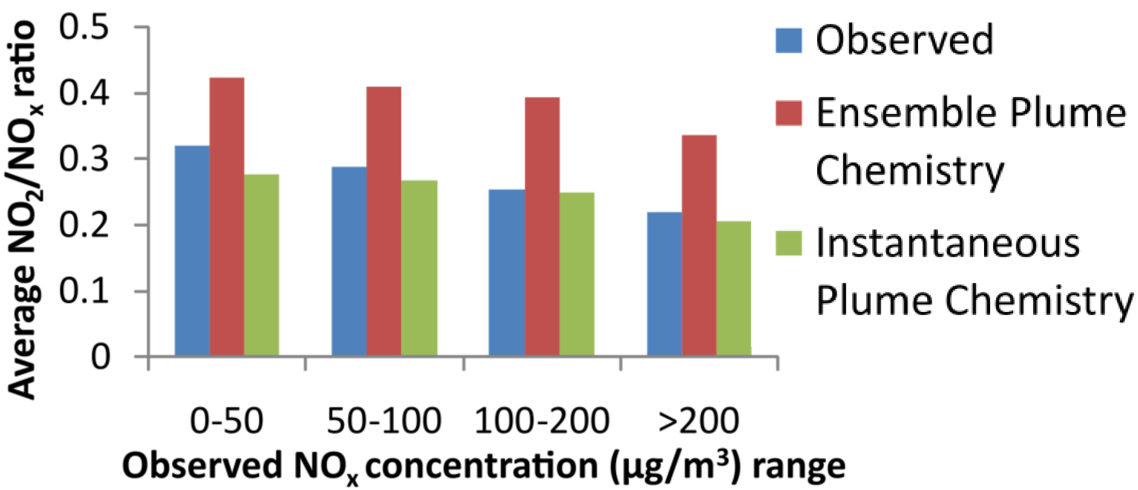


Validation

Case study: Wainwright – NO_2/NO_x ratios

- Comparing NO_2/NO_x ratios gives good indication of chemistry performance
- Time-paired comparisons
- Instantaneous plume chemistry compares better with observed NO_2/NO_x

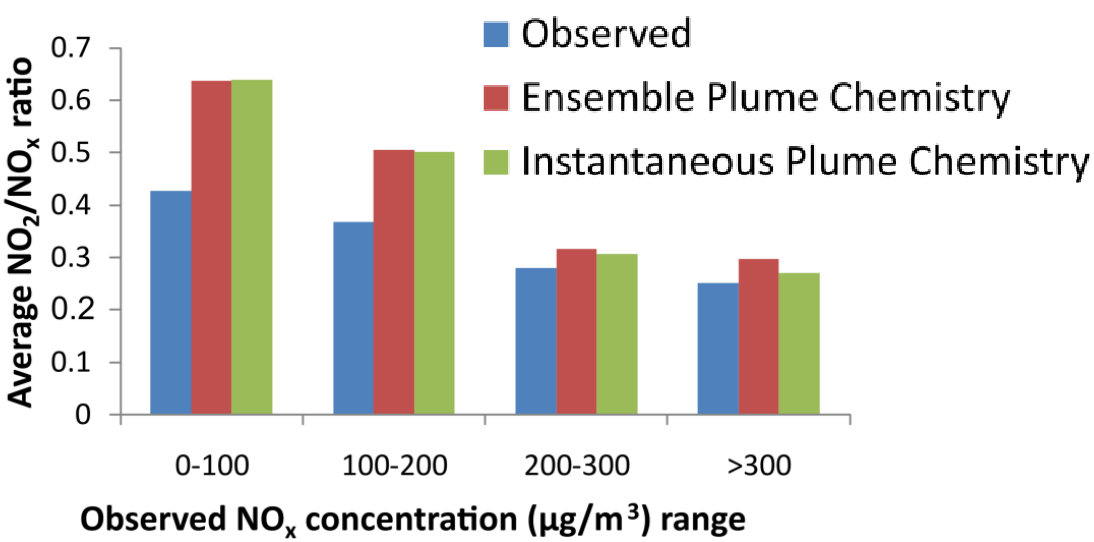


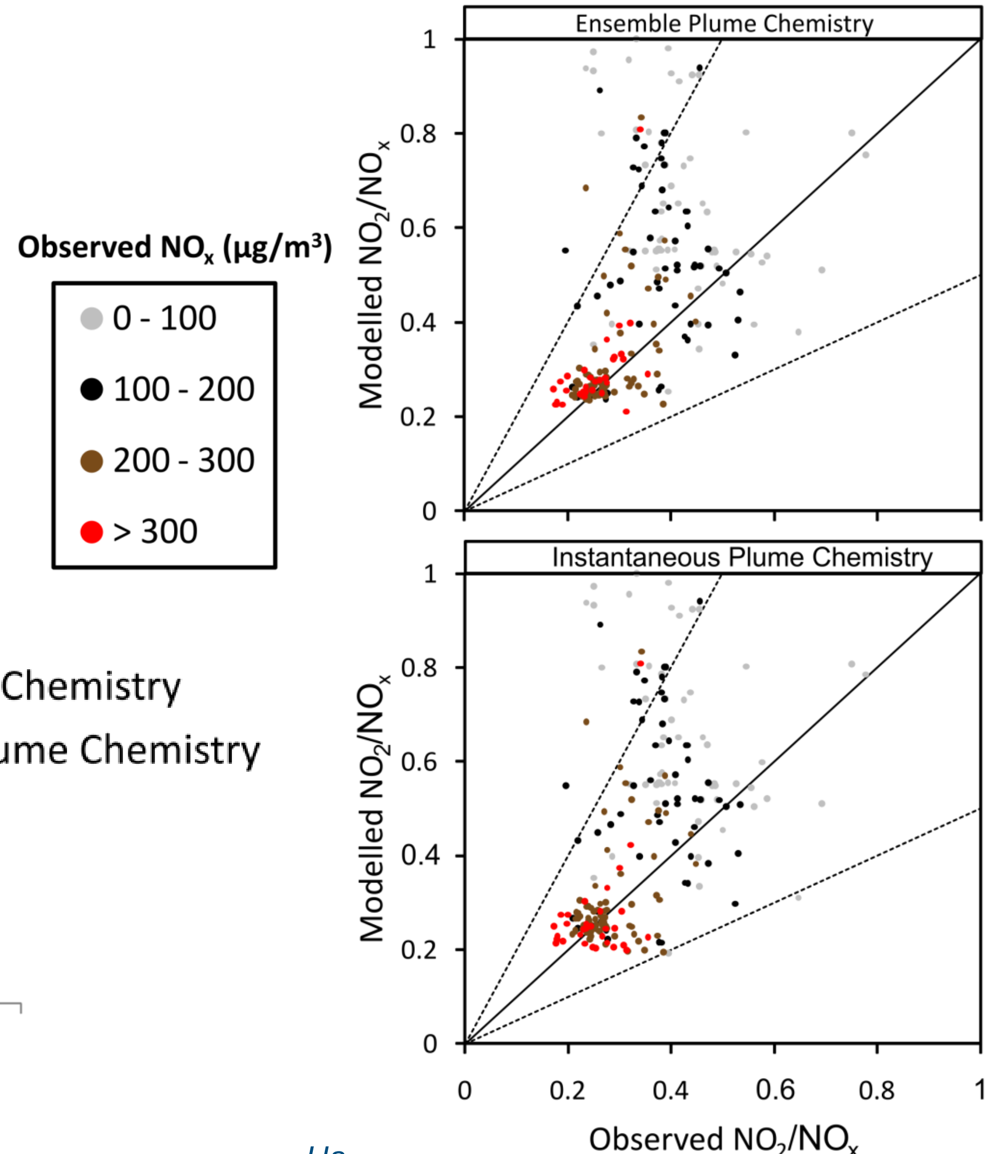


Validation

Case study: Prudhoe Bay – NO_2/NO_x ratios

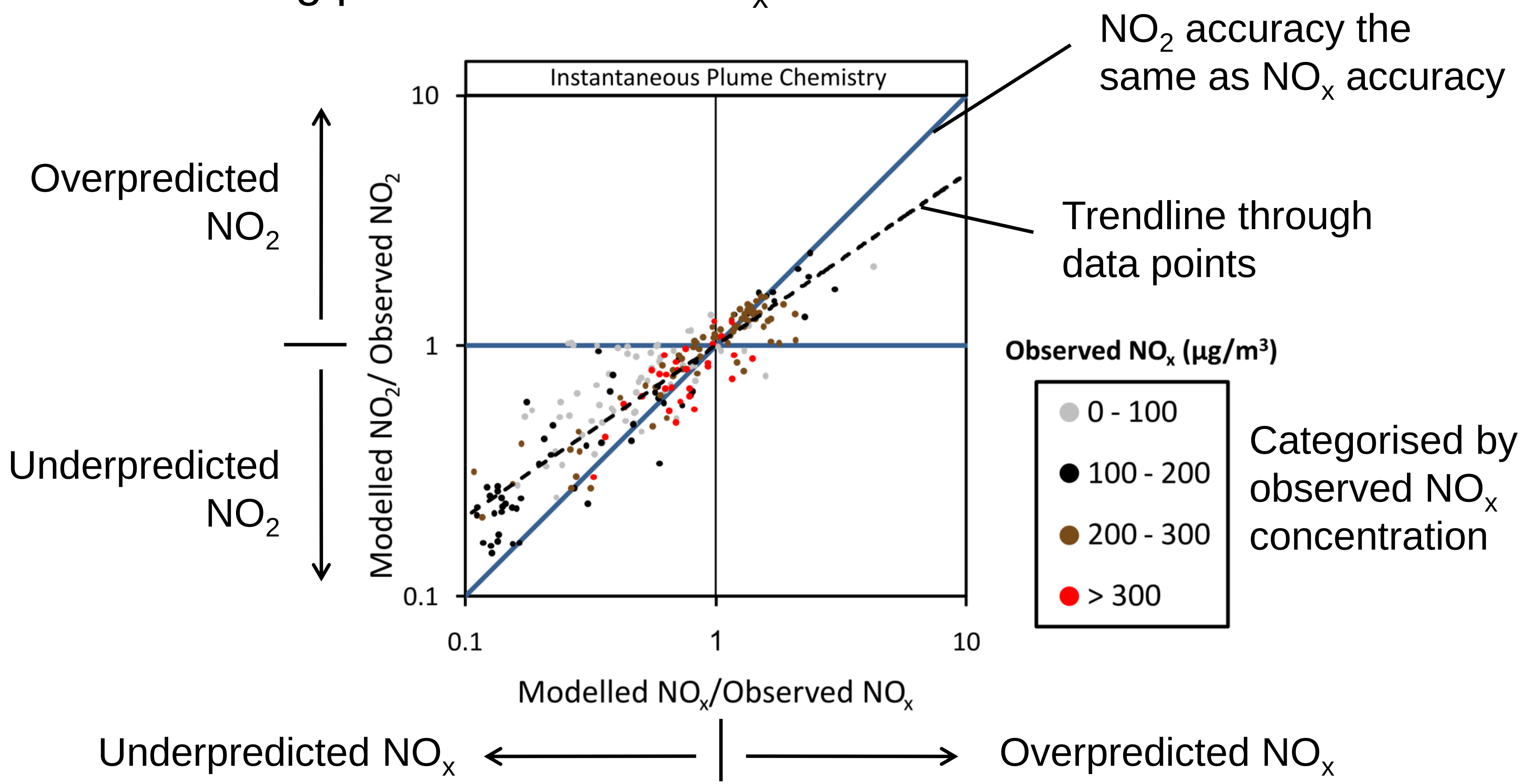
- Two chemistry schemes perform similarly
- Instantaneous plume chemistry predicts slightly more accurate NO_2/NO_x
- Better prediction for higher NO_x concentrations





Comparing modelled/observed ratios

- Insightful to compare modelling performance of NO_2 to modelling performance of NO_x

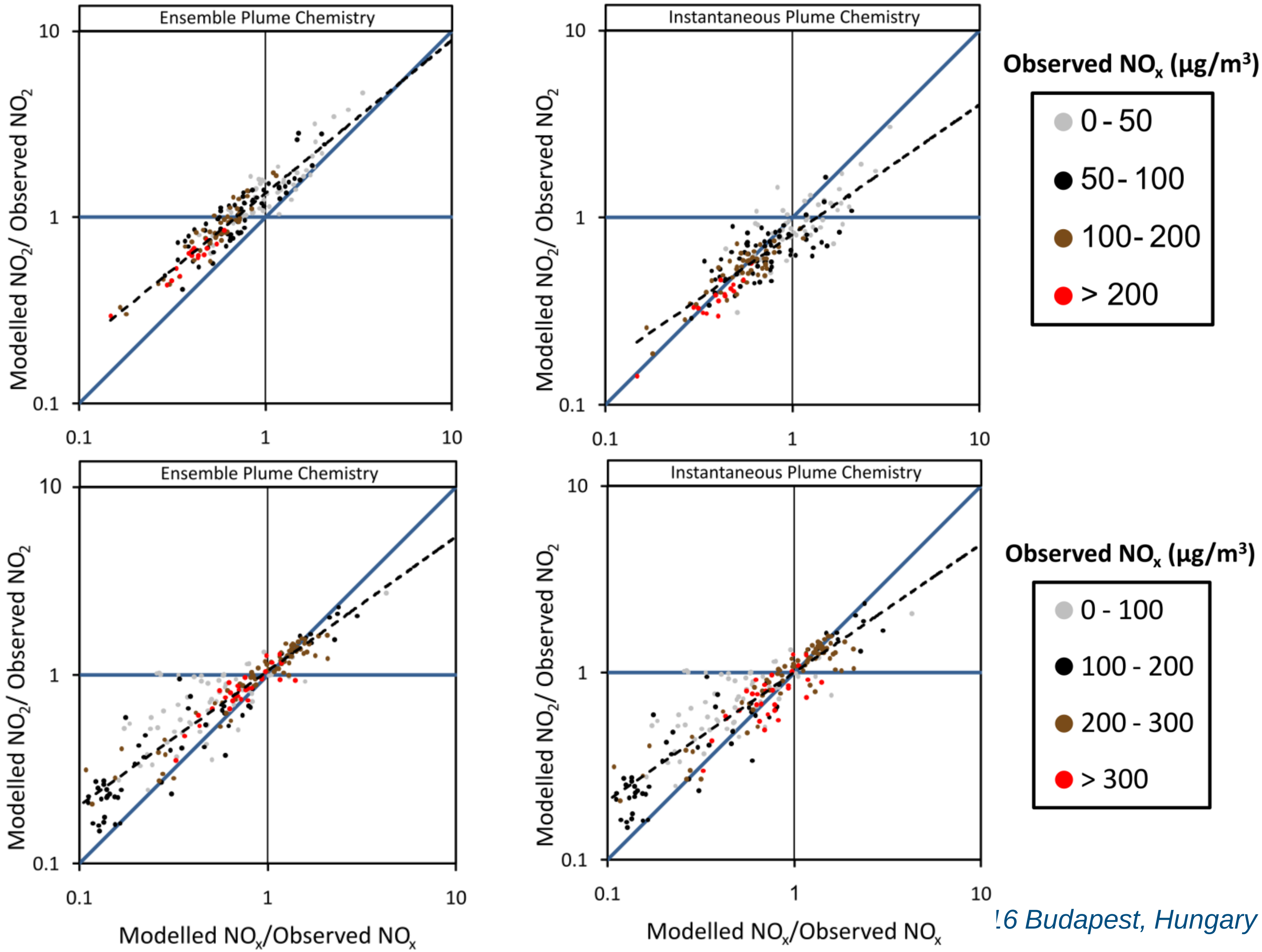


Case studies: Results

Ensemble NO_2 | Instantaneous NO_2

Wainwright

Prudhoe Bay



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Summary

- ADMS NO_x chemistry validation for two schemes using two Alaskan case studies
- NO_2 model performance considered in the context of NO_x model performance
  - Concentrations, NO_2/NO_x ratios and modelled/observed ratios were used to determine performance of chemistry models
- Both chemistry schemes compared well for both case studies
  - Ensemble plume chemistry predicted higher NO_2 concentrations than instantaneous plume chemistry
  - Instantaneous plume chemistry NO_2 concentrations compared better to measurements, when considered alongside modelled NO_x performance

Thank you for listening

Any questions?