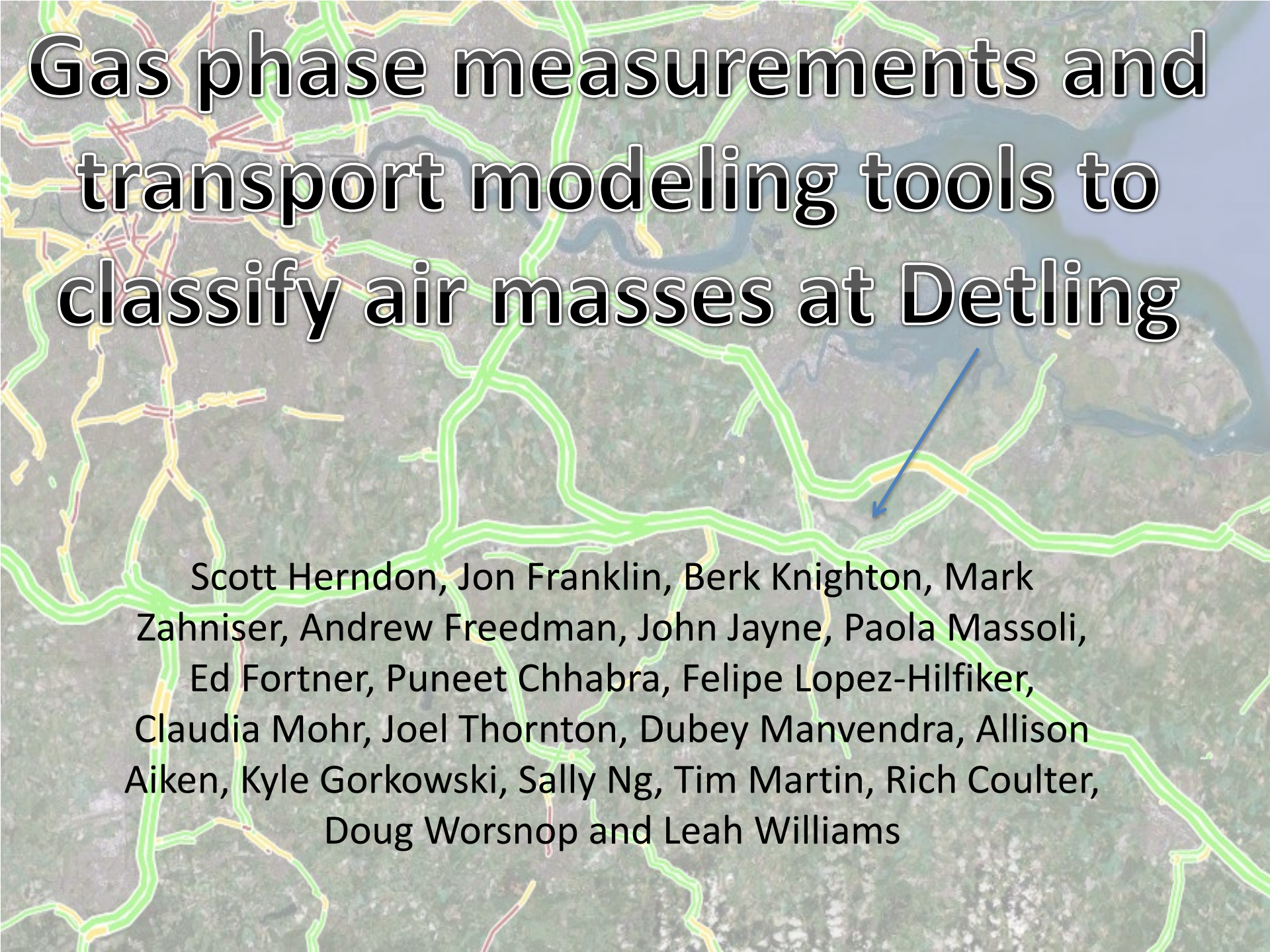
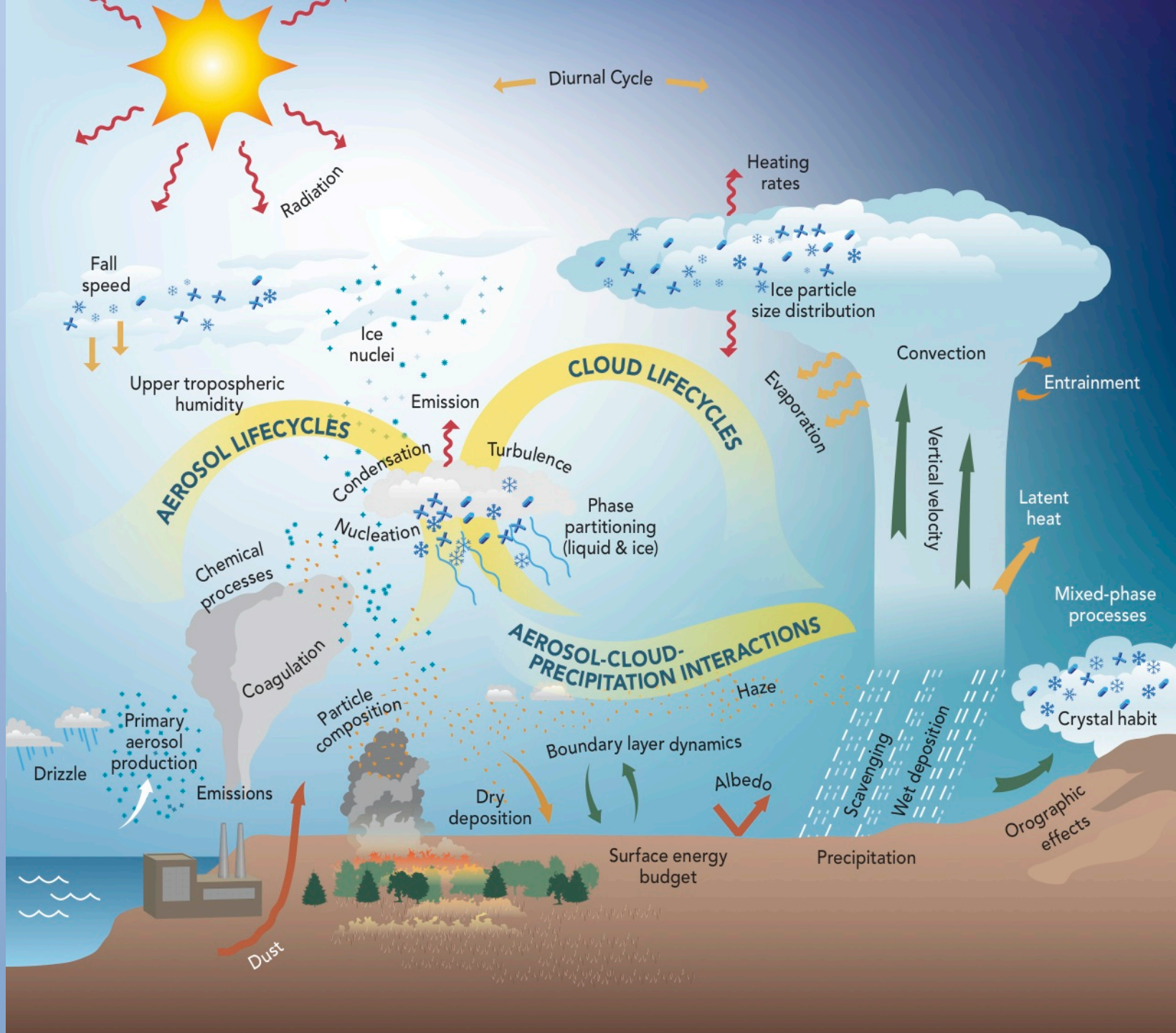
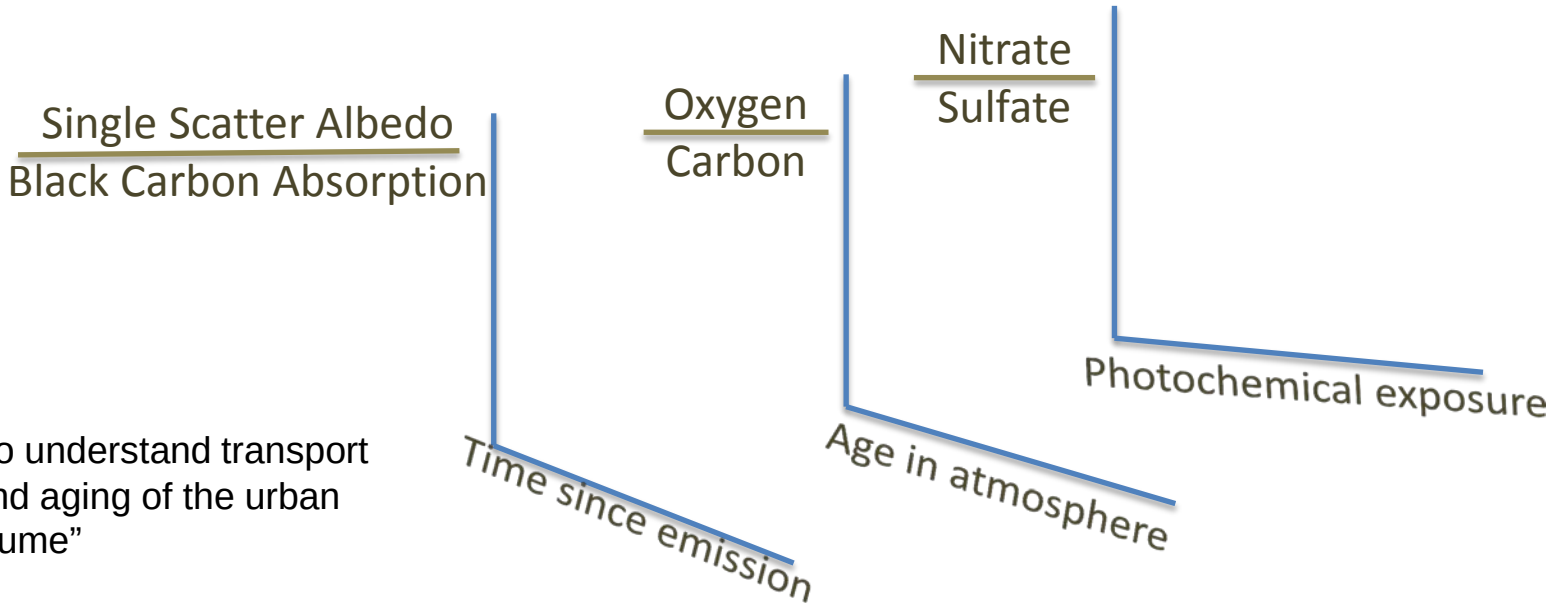
Gas phase measurements and transport modeling tools to classify air masses at Detling



Scott Herndon, Jon Franklin, Berk Knighton, Mark Zahniser, Andrew Freedman, John Jayne, Paola Massoli, Ed Fortner, Puneet Chhabra, Felipe Lopez-Hilfiker, Claudia Mohr, Joel Thornton, Dubey Manvendra, Allison Aiken, Kyle Gorkowski, Sally Ng, Tim Martin, Rich Coulter, Doug Worsnop and Leah Williams


Diurnal Cycle
Radiation
Heating rates
Ice particle size distribution
Fall speed
Ice nuclei
Upper tropospheric humidity
Emission
CLOUD LIFECYCLES
AEROSOL LIFECYCLES
Condensation
Turbulence
Nucleation
Phase partitioning (liquid & ice)
Chemical processes
Coagulation
Evaporation
Convection
Entrainment
Vertical velocity
Latent heat
Mixed-phase processes
AEROSOL-CLOUD-PRECIPITATION INTERACTIONS
Haze
Crystal habit
Primary aerosol production
Drizzle
Emissions
Particle composition
Boundary layer dynamics
Dry deposition
Albedo
Scavenging
Wet deposition
Orographic effects
Surface energy budget
Precipitation
Dust

Independent determination of *time*

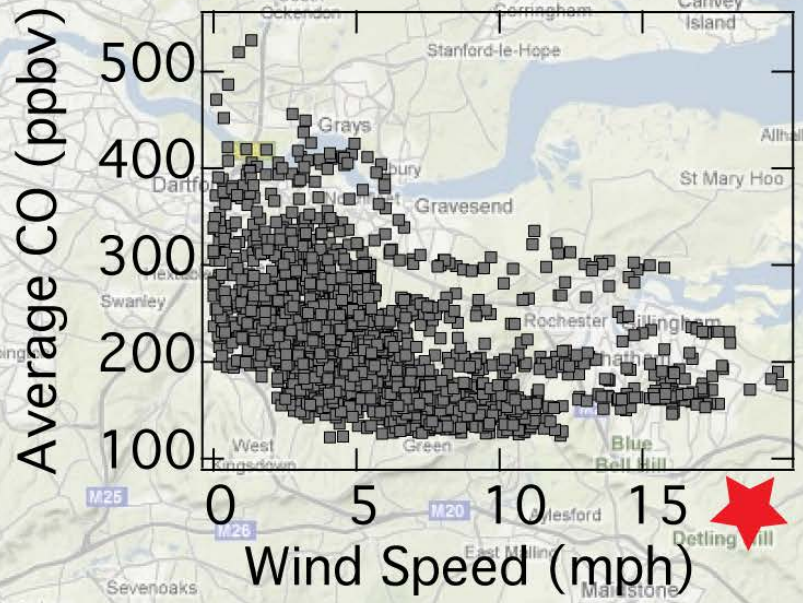


"to understand transport and aging of the urban plume"

Gas phase measurements and transport modeling tools to evaluate *time* in the context of aerosol processing

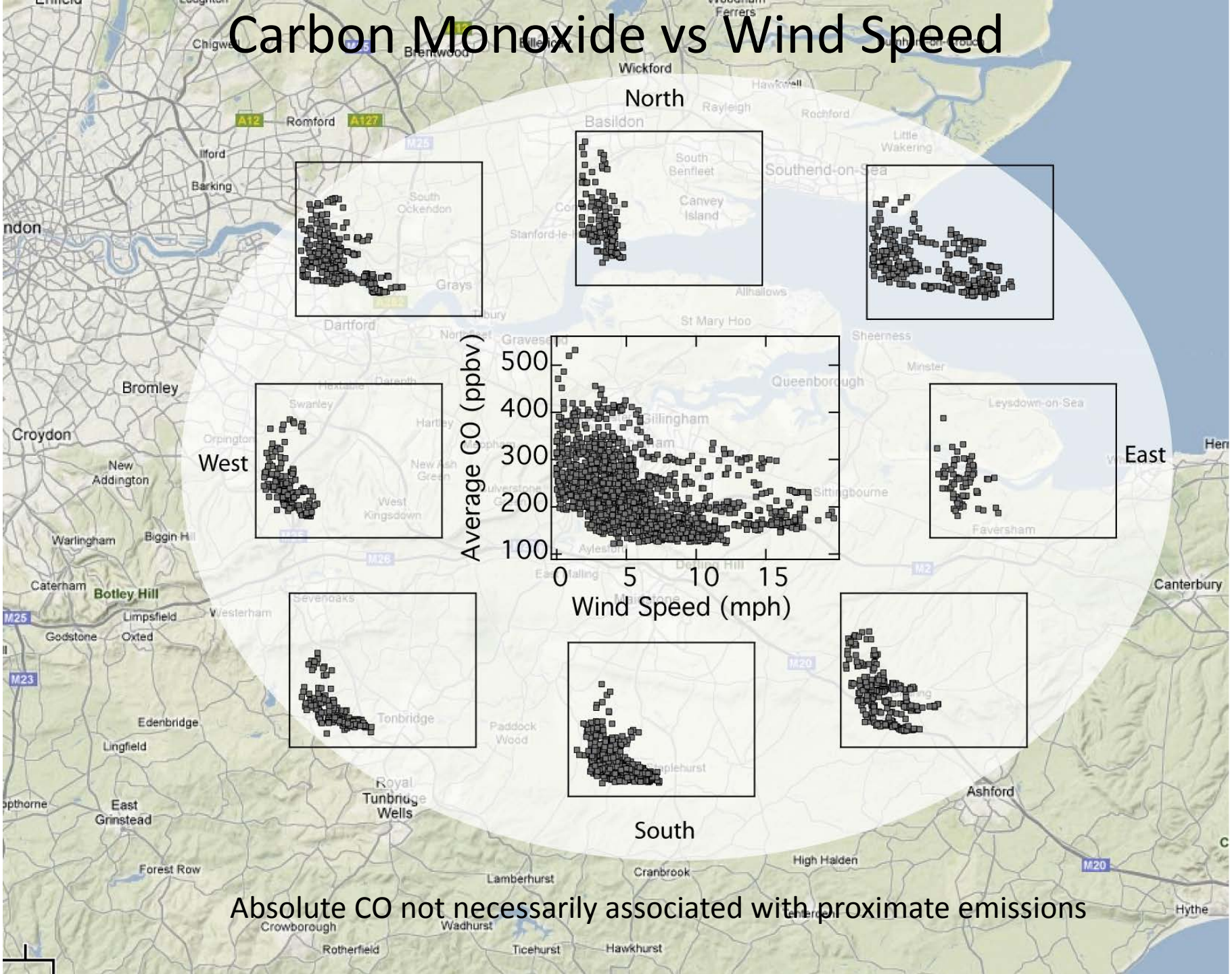
① Carbon Monoxide variability
② HYSPLIT
③ Photochemical Clock via aromatic ratios
④ Putting it together and Future Steps

Carbon Monoxide vs Wind Speed



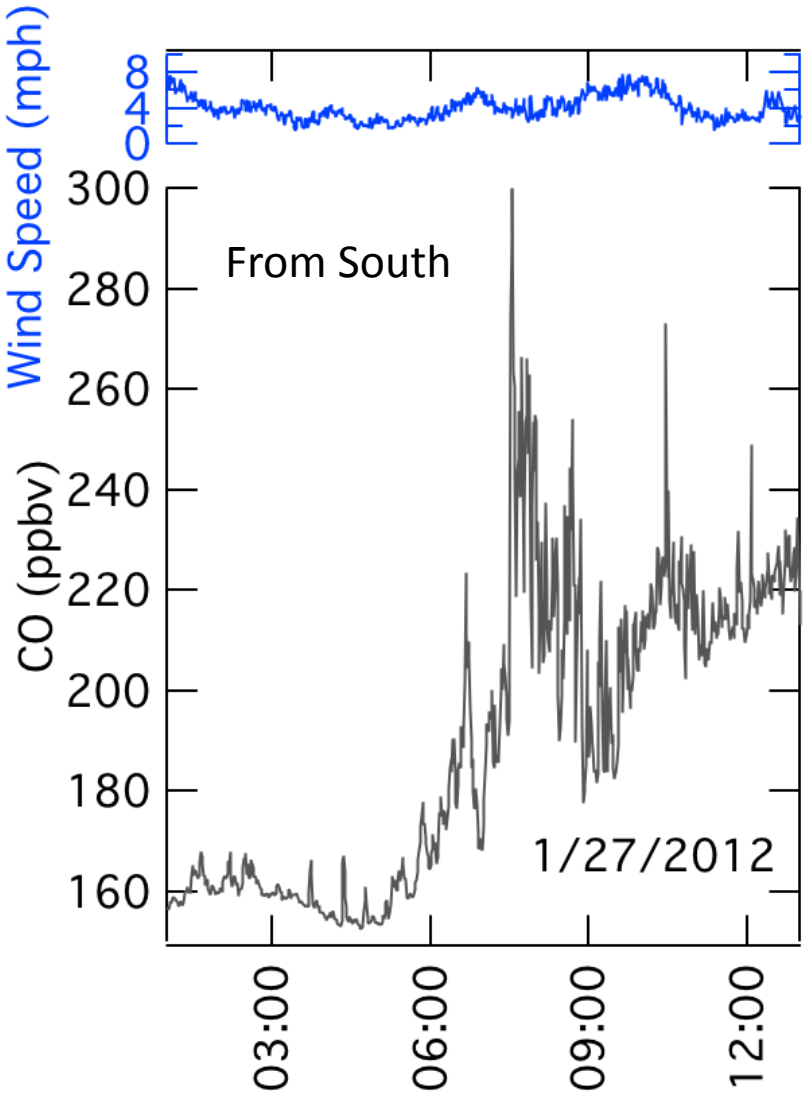
(1) CO Variability

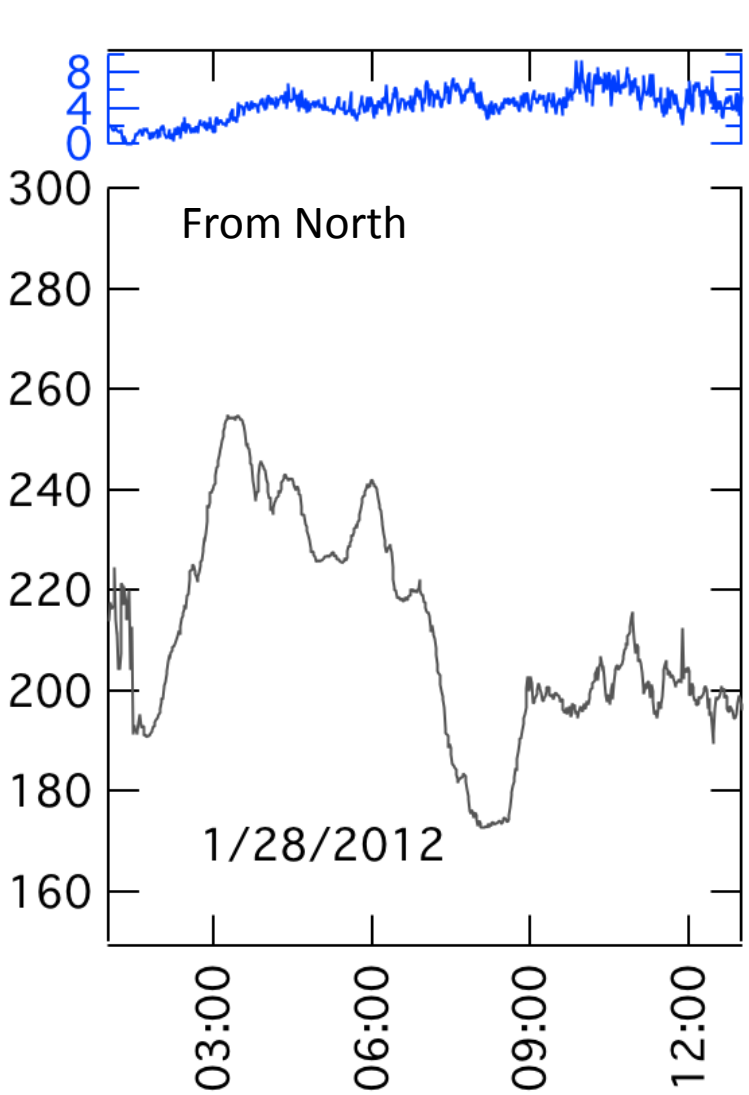
Carbon Monoxide vs Wind Speed



Absolute CO not necessarily associated with proximate emissions

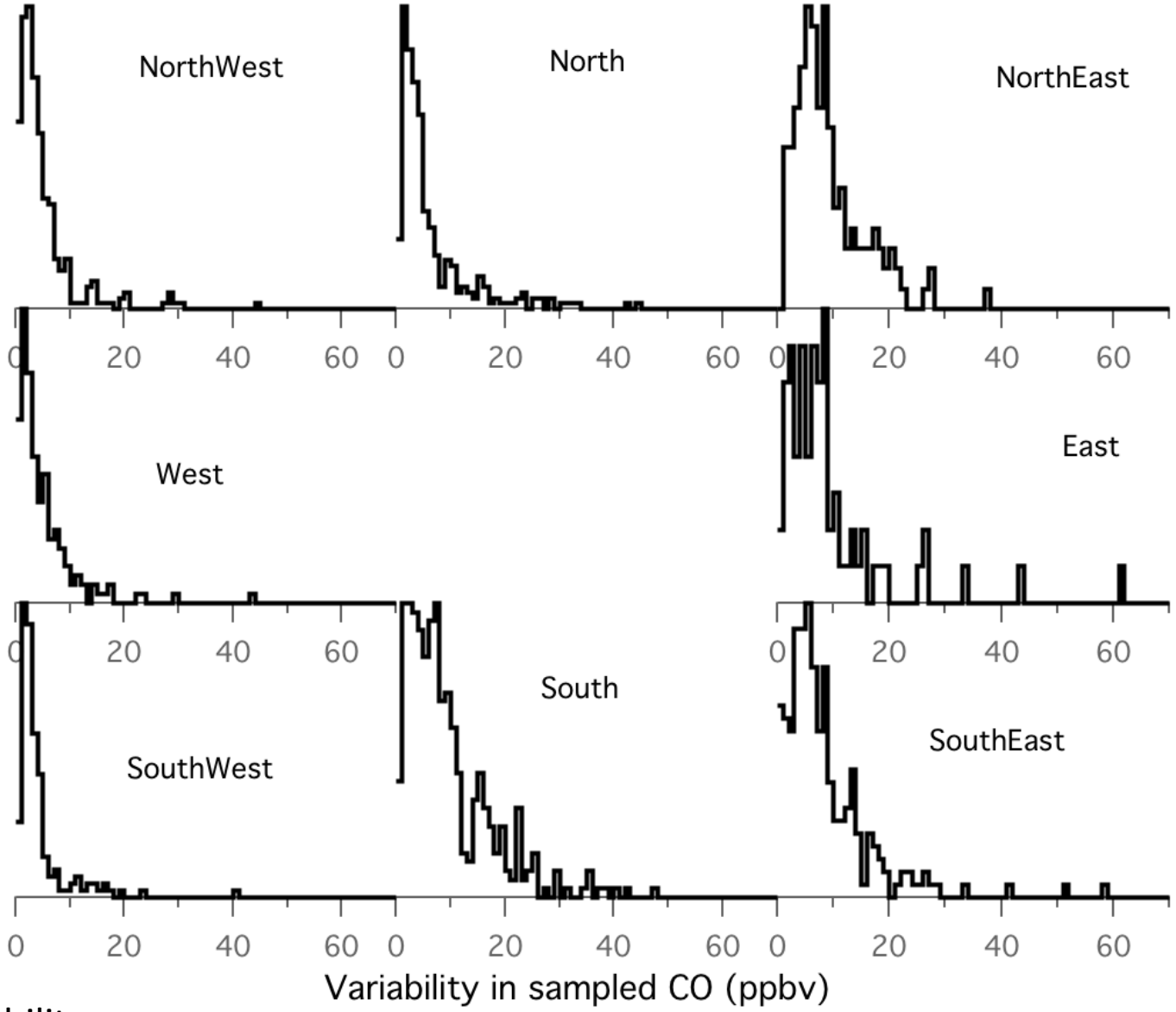
Can CO variability be more indicative of proximity?





(1) CO Variability

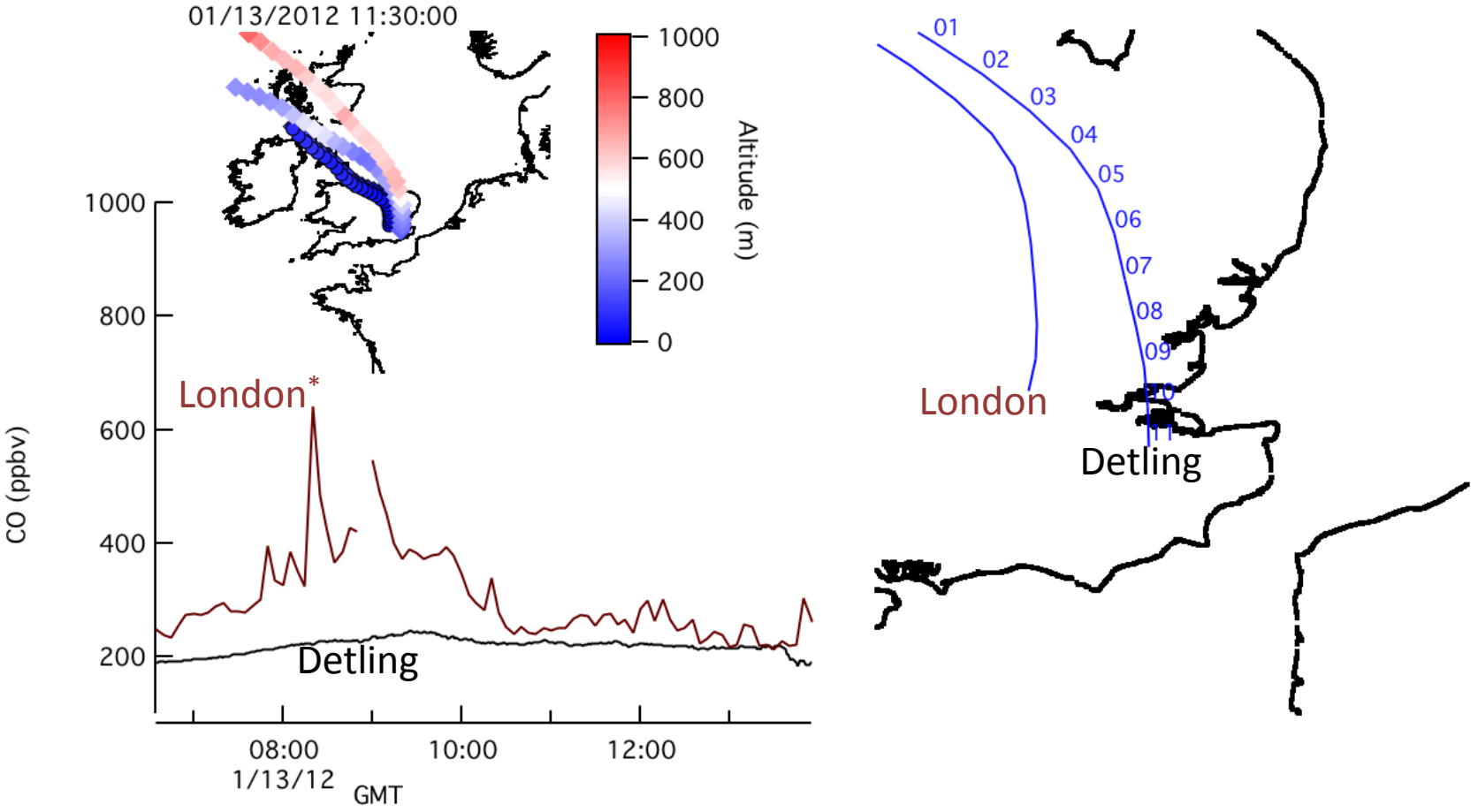
Can CO variability be more indicative of proximity?



(1) CO Variability

HYSPLIT

Hybrid Single Particle Lagrangian Integrated Trajectory

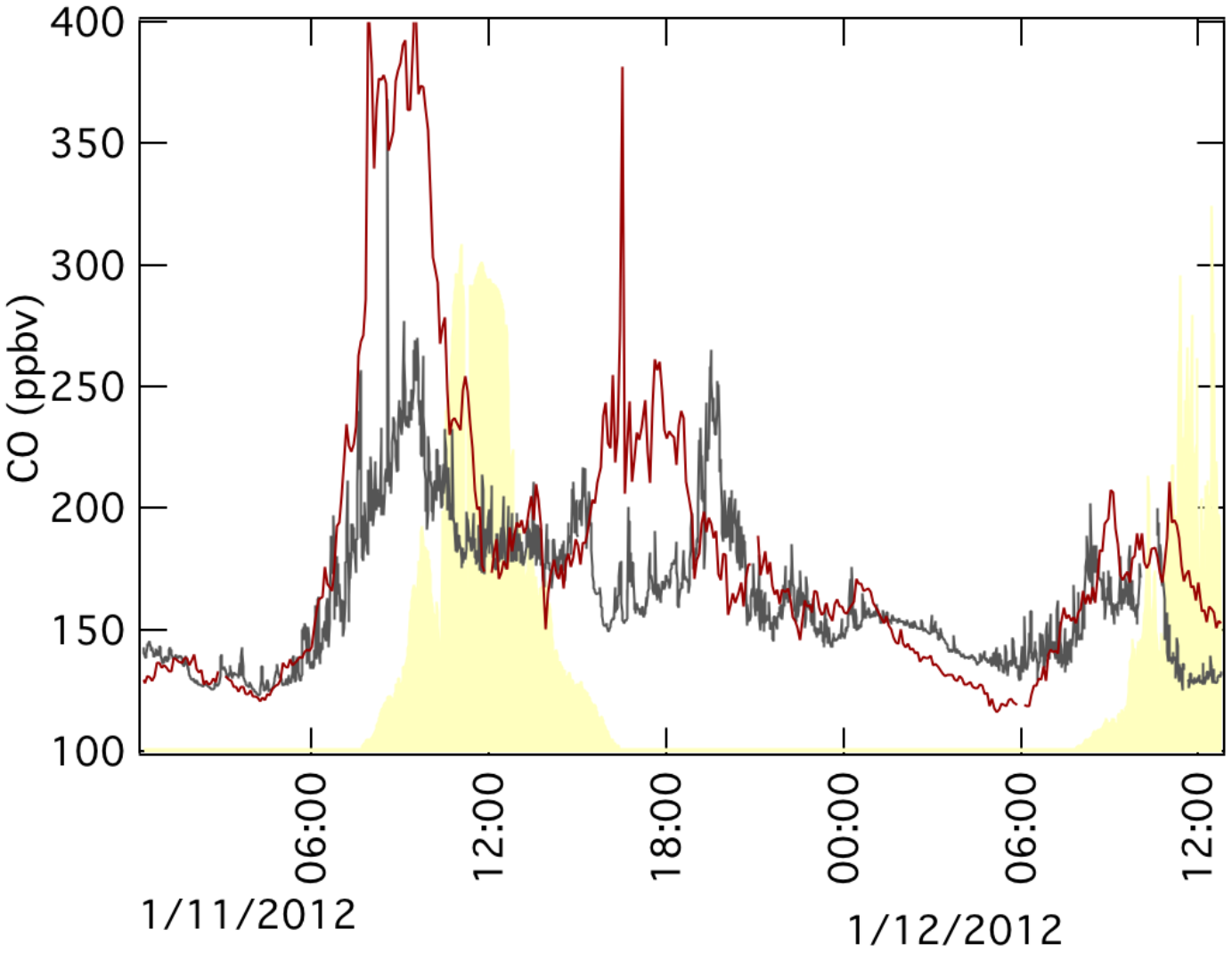


*North Kensington CO data from James Lee

HYSPLIT Citations: Draxler, R.R., and G.D. Hess, 1997: Description of the HYSPLIT_4 modeling system. NOAA Tech. Memo. ERL ARL-224, NOAA Air Resources Laboratory, Silver Spring, MD, 24 pp. and Rolph, G.D., 2012. Real-time Environmental Applications and Display sYstem (READY) Website (http://ready.arl.noaa.gov). NOAA Air Resources Laboratory, Silver Spring, MD.

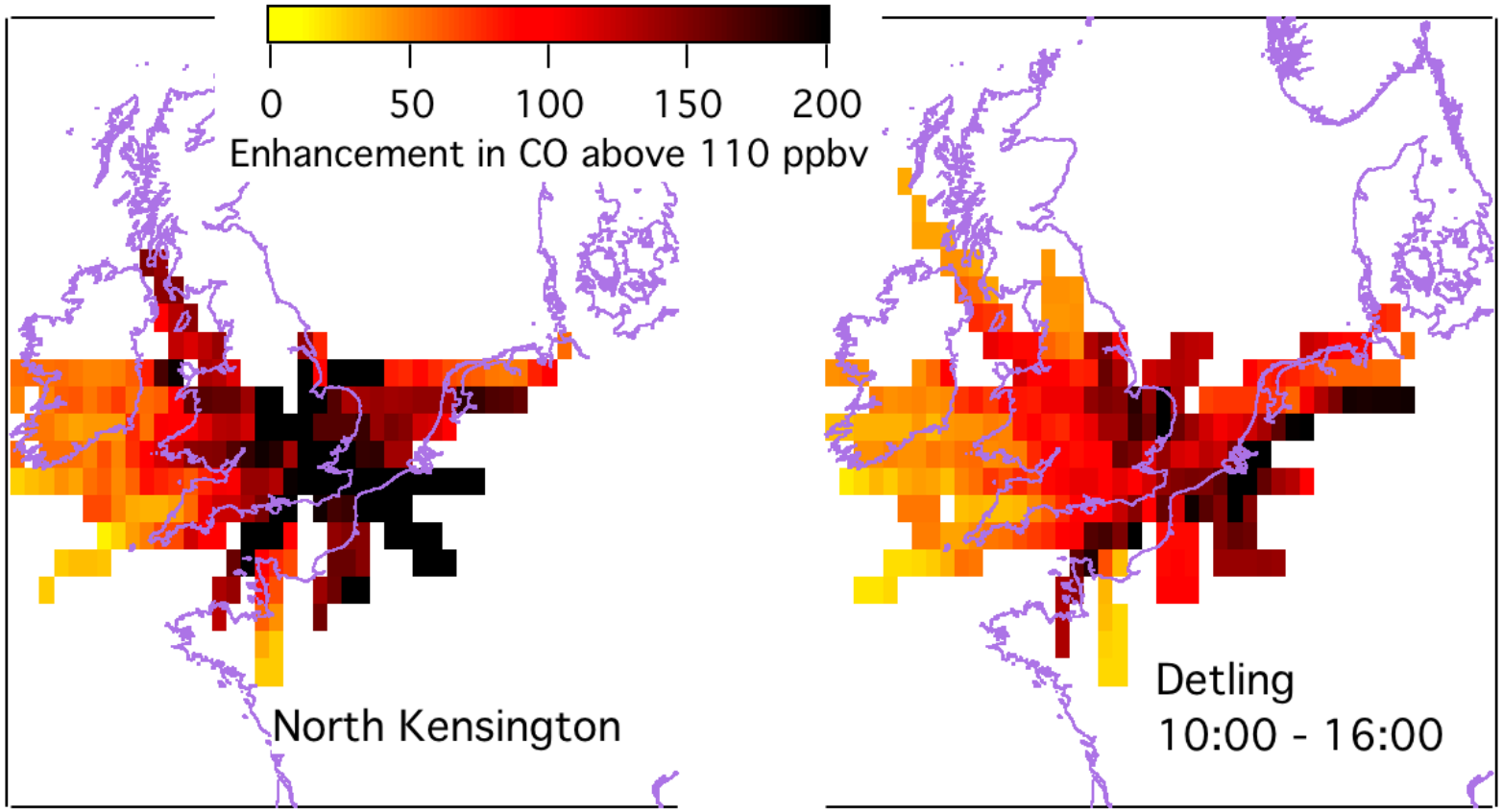
(2) Transport Calculations

London vs Detling



(2) Transport Calculations

Spatial average along back-trajectory



CO elevated due to transport from Northern Europe relative to transport from Atlantic

(2) Transport Calculations

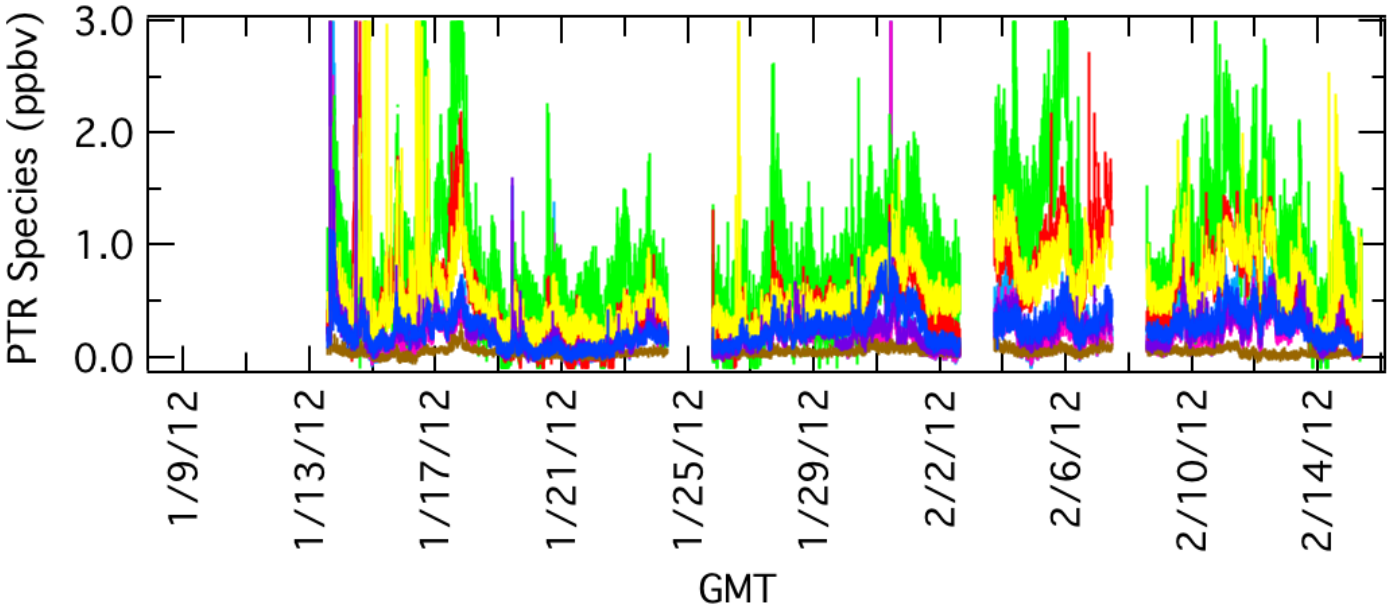
Photochemical Clock using VOC Ratios

$$\Delta t\,[OH] = 1/(k_{VOC} - k_{benzene})\,[\ \ln\{VOC_0/Benzene_0\} - \ln\{VOC_t/Benzene_t\}\ ]$$

Emission Ratio

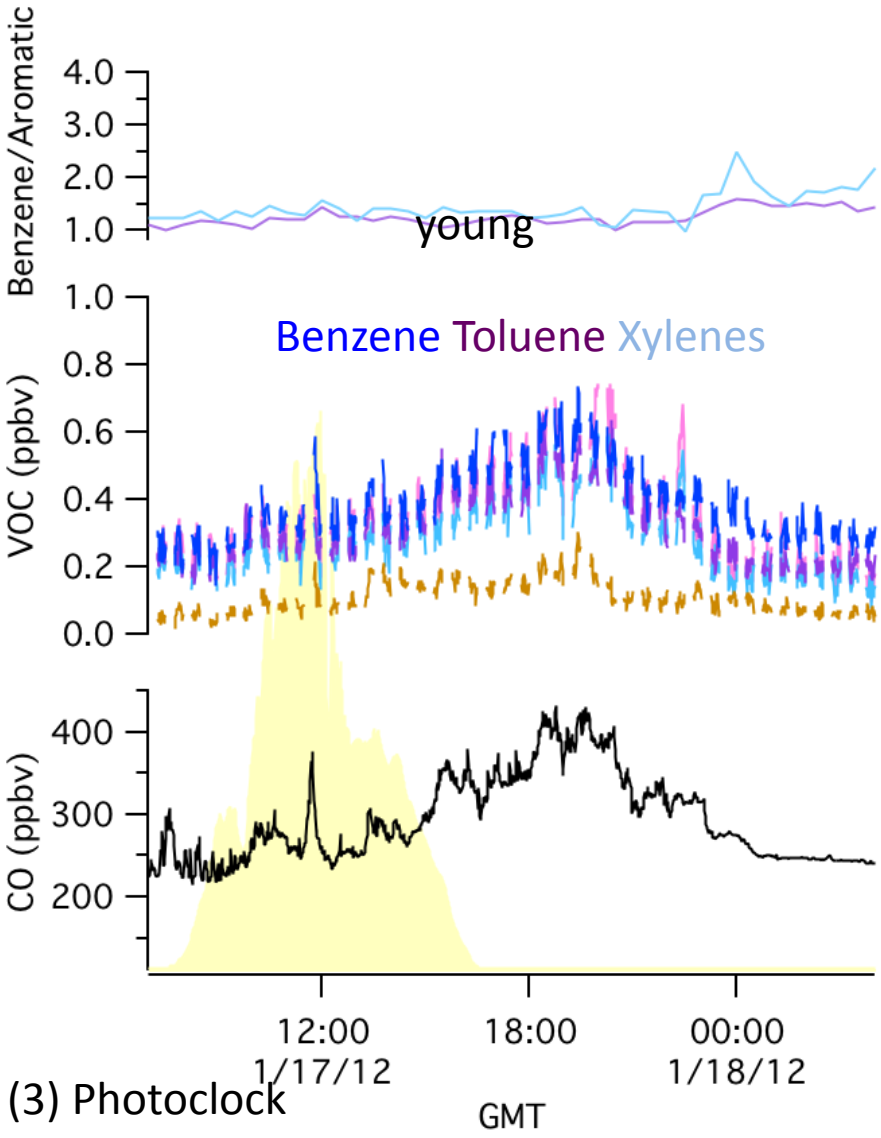
Measured Ratio

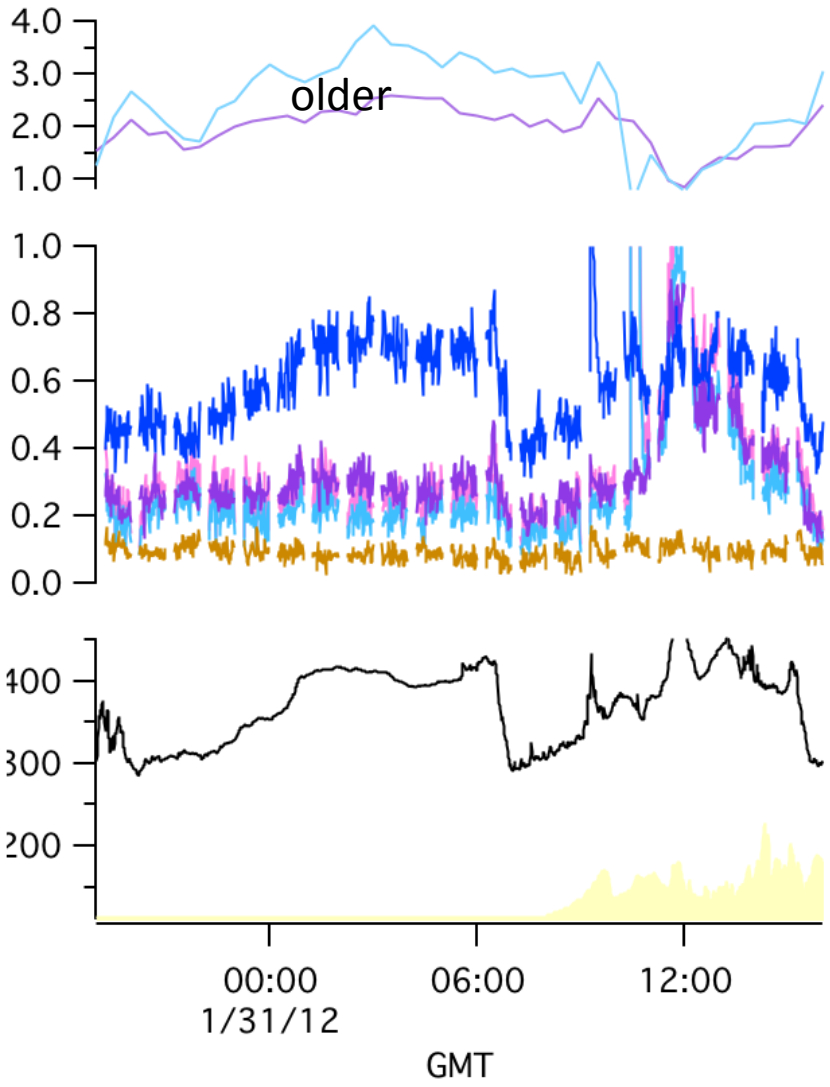
Mixing time scale couples with advection time scale. What does Δ*t* mean?



Knighton PTR data

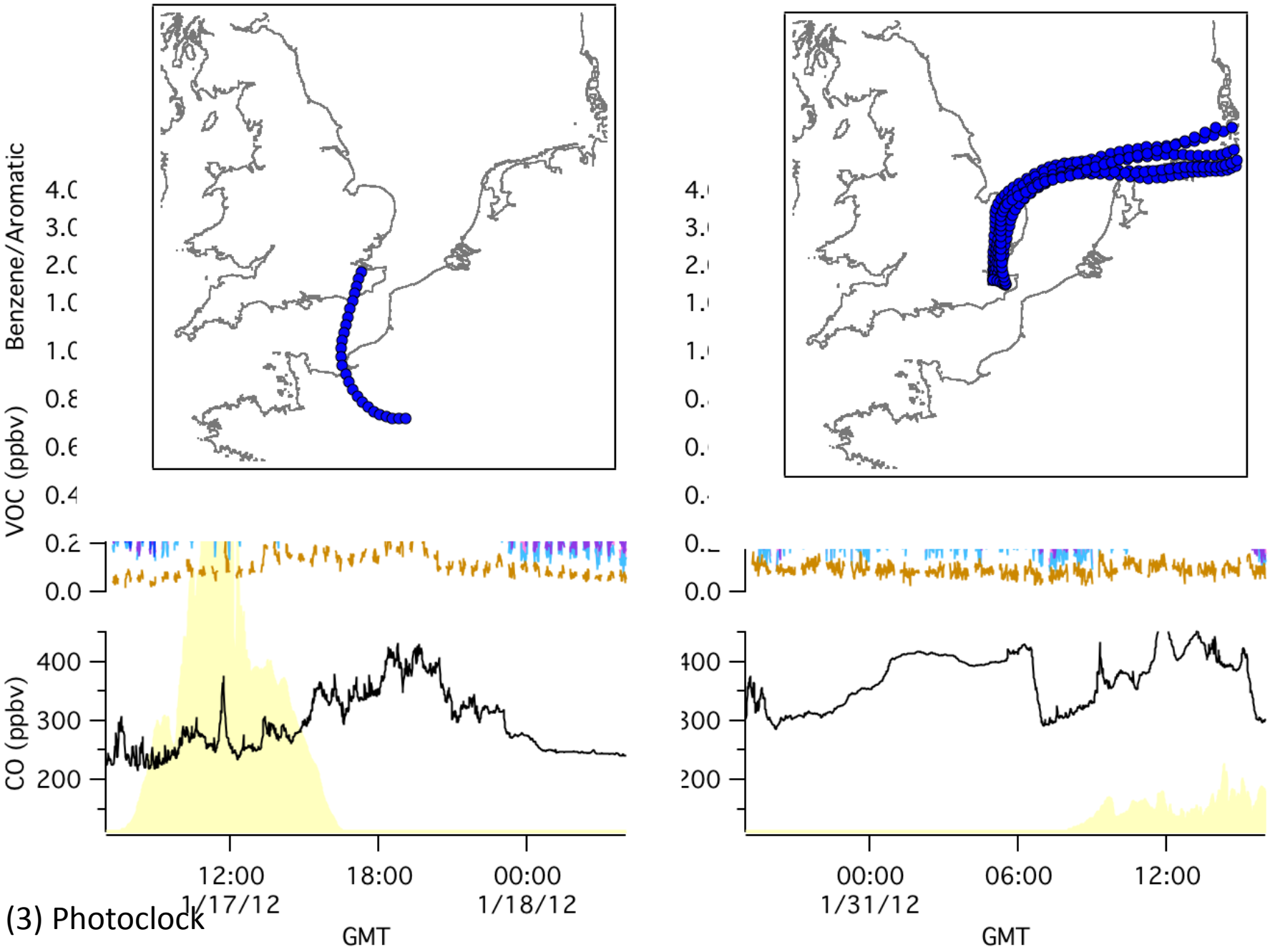
Benzene to Toluene





(3) Photoclock

HYSPLIT and VOC Clock



(3) Photoclock

Summary

- Measured CO variability can be used to signal “close” emissions
- Greater CO mixing ratios are not necessarily “close” CO

- HYSPLIT is adequate to help qualitatively assign transport
  - London and Detling have same CO when transport brings Atlantic airmass to Southern England
- Benzene/Aromatic “Clock” can constrain transport scale, maybe

Future Work

- Verify local wind with ANL and assimilate nearby real wind data
- Produce quantitative vector representing emissions from road(s)
- Attribute CO -> remote, European transport, London outflow
- Couple these representations of mixing and processing *time* with PM properties

gas phase measurements at Detling

Long-lived airmass tracer compounds:
- carbon monoxide (CO)
- carbon dioxide (CO_2)
- methane (CH_4)
- nitrous oxide (N_2O)

- sulfur dioxide (SO_2)

Oxides of nitrogen and ozone:
- ozone (O_3)
- nitric oxide (NO)
- nitrogen dioxide (NO_2)
- nitryl chloride ($ClNO_2$)
- dinitrogen pentoxide (N_2O_5)
- total NO_y <= *Thanks David!*

Hydrocarbons:
- benzene, toluene, other aromatics

- acetonitrile
- methanol
- isoprene, alpha pinene

- formaldehyde, acetaldehyde, acetone
- methyl vinyl ketone, methacrolein

GC-FID Hydrocarbons:
- TENAX preconcentration
- C5+