Ozone and Air Quality

Some Selected Research Projects in the Chemical Sciences Division



Joost de Gouw & Christoph Senff



- 1. Research approach and tools
- 2. Ozone precursor emissions
- 3. Nighttime chemical transformation
- 4. Land-sea breeze circulation
- 5. Ozone regional transport
- 6. Nighttime transport in low-level jet

- Joost

Christoph

Ozone - Air Quality Research in CSD



- Interplay between different approaches is one of the keys to success
- Collaboration with GSD and PSD on (forecasting) models
- Collaboration with GMD on ozone measurements

Tools for Field Measurements Used by CSD



In-situ Measurements (WP-3 and Ron Brown) Ozone precursors and radiation Radicals By-products of ozone chemistry

<u>Remote Measurements</u> (Twin Otter and Ron Brown) Ozone lidar Doppler wind lidar



ESRL Regional Air Quality Field Studies



VOC Emissions from Petrochemical Industries





Houston has a severe ozone problem due to emissions from the petrochemical industry

NOAA performed the Texas Air Quality Studies in 2000 and 2006

Work by: Joost de Gouw, Carsten Warneke, Tom Ryerson

Ethene Emissions From Industrial Point Sources



 TexAQS 2000: Ethene is one of the main reactive VOCs
 A laser photo-acoustic instrument was developed for fast-response measurements during TexAQS 2006

Ethene Emissions From Industrial Point Sources



Ethene flux from Freeport:



Emissions are severely underestimated in inventories developed by the State of Texas

As a result, rapid ozone production in industrial plumes is underestimated by models

Verification of Isoprene Emissions Inventories



Isoprene: large sources ~35% of all VOC emissions high reactivity midday lifetime <1 hour
 Reliable estimates of the emissions is key in ozone models

Work by: Carsten Warneke, Joost de Gouw

Validation of Isoprene Emission Inventories



Warneke et al. [in preparation]

 Inventories constructed from land-use data and emission factors depending on vegetation type
 Here: validate U.S. emission inventories using aircraft data

Validation of Isoprene Emission Inventories

Example from 1 research flight over NE Texas:

35 OK AR 34 33 LA 32 TΧ 31 500 30. isoprene (pptv) 29 -98 -96 -94 -92 -90



Warneke et al. [in preparation]

NOAA WP-3

Measurements:
➤ 1-sec PTR-MS data
➤ Scatter due to real atmospheric variability

Model:
➢ EPA BEIS3.13 inventory
➢ ECMWF temperature and radiation

Measurements agree with inventory within factor of ~2

Nighttime Chemical Processing

Work by: Steve Brown, Bill Dubé, Hendrik Fuchs, Roberto Sommariva

Diurnal Nitrogen Oxide Cycles



 NO_x , VOC , O_3 transformed at night

Vertical Stratification & Nighttime Chemistry



NOAA WP-3

- NO_x and VOC plumes occur in discrete layers at night
- Chemical transformation within different layers differs markedly



Boundary Layer Vertical Profiles Erie (BAO) Tower

- 300 m w/ vertical resolution ~ 0.5 m
- Movable carriage on *outside* with > 1 ton payload



• Studies in 2004 (fall) and 2007 (summer)



- High NO₃ routinely observed aloft
- Often associated with complex layering

Surface layer commonly observed

Ozone Transport and Mixing Processes

• Local-scale transport:

Land – sea breeze circulation in Houston, TX

Regional transport:

Increasingly important as 8-hour O₃ standards are tightened

• Nighttime processes:

Transport and mixing by low-level jet

Ozone Lidar:

TOPAZ = Tunable Optical Profiler for Aerosol and Ozone



TOPAZ lidar mounted in NOAA Twin Otter

R. Alvarez II, C. Senff, et al.





Ozone profiles & mixed layer height

Doppler Wind Lidar:

HRDL = High Resolution Doppler Lidar



S. Tucker, A. Brewer, et al.





Wind speed & direction profiles

Wind Profiler Network (PSD):





NOAA/ESRL Integrated Wind Profiler Observing Site

TEXAQS-II East Texas Wind Profiler Network

A. White et al.

Wind Profiler Network (PSD):



TEXAQS-II East Texas Wind Profiler Network



A. White et al.

Local Transport: Houston land-sea breeze recirculation



Air Quality forecast model comparison with lidar



Lidar O₃ cross section

MM5/Chem model (1.7 km horizontal resolution)

J.-W. Bao, G. Grell, S. McKeen

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Regional Transport: Estimating ozone exported from Houston



Regional Transport: Houston Ozone Flux



A flux of 35 kg O_3 s⁻¹ transported out of Houston over an 8-hour day is equivalent to a 10-ppb increase in ozone over an approx. 10,000 square mile area, assuming a 2-km deep mixed layer.

Nighttime Transport & Mixing



12-hour forward trajectories: 6 PM – 6 AM LST

- Nighttime low level jet can transport O₃ over long distances.
- Speed and directional wind shear at night are very effective in distributing O₃ over large areas.

Nighttime Transport & Mixing





Wind speed variance: $\sigma_u^2 \approx TKE$





R. Banta, Y. Pichugina, et al.

Summary: Ozone - Air Quality Research in CSD



Atmospheric measurements of emissions, chemical and dynamical processes are an important cornerstone.

Laboratory measurements and modeling studies complete CSD's ozone – air quality research approach.