HOx Photochemistry during DC3

Abstract # A41B-0040

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Experimental

- Campaign: Deep Convective Clouds and Chemistry (DC3)
- Location: Salina, Kasas
- Period: May-June, 2012
- Platform: DC-8
- Instruments:
  - Airborne Tropospheric Hydrogen Oxides Sensor (ATHOS) for OH and HO_2 detection based on laser-induced fluorescence (LIF), detection limits: OH = 0.01 pptv; HO_2 = 0.1 pptv; uncertainty: ~±40% (2σ confidence).
  - Airborne OH Reactivity Instrument: 20-s time resolution; uncertainty: ~±1 s^{-1} (2σ confidence).

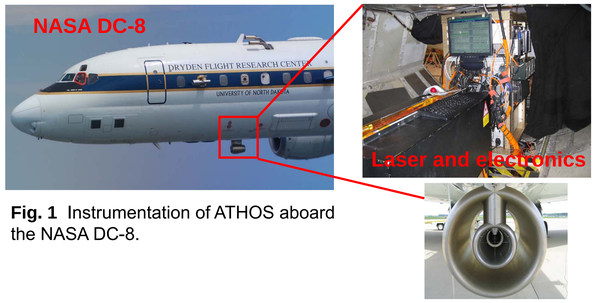


Fig. 1 Instrumentation of ATHOS aboard the NASA DC-8.

Model Calculations

RACM2 photochemical box model (Goliff et al., AE, 2013) constrained by observed data (DC8 1-min merged data Version R3) of O_3, CO, NO, NO_2, SO_2, H_2O_2, VOCs (including alkanes, alkenes, aromatics, carbonyls, PAN and other organic nitrates), photolysis frequencies, T, P and humidity. Model output includes time series of OH, HO_2, RO_2, and other reactive intermediates.

Observation Results

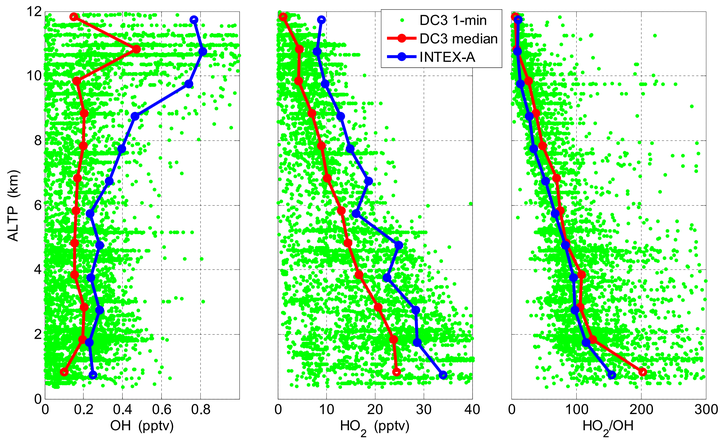


Fig. 2 Vertical profiles of observed OH, HO_2, and HO_2/OH during DC3. For comparison, the same vertical profiles are plotted for flights out of the St. Louis area during INTEX-A.

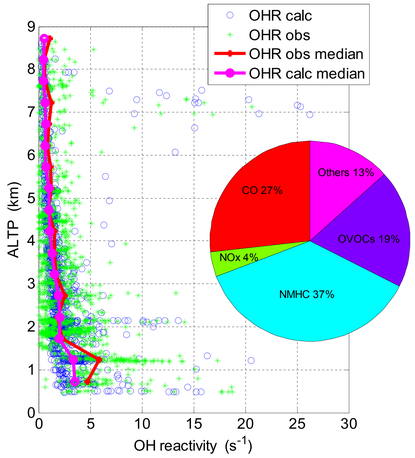


Fig. 3 Vertical profiles of observed and calculated OH reactivity during DC3. Pie chart shows the contributions to OHR from observed OH reactants.

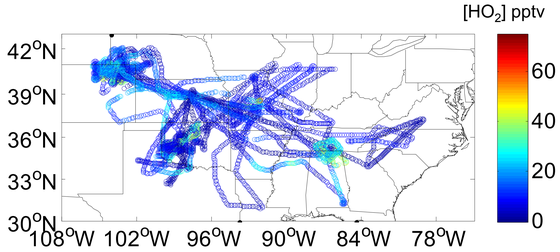
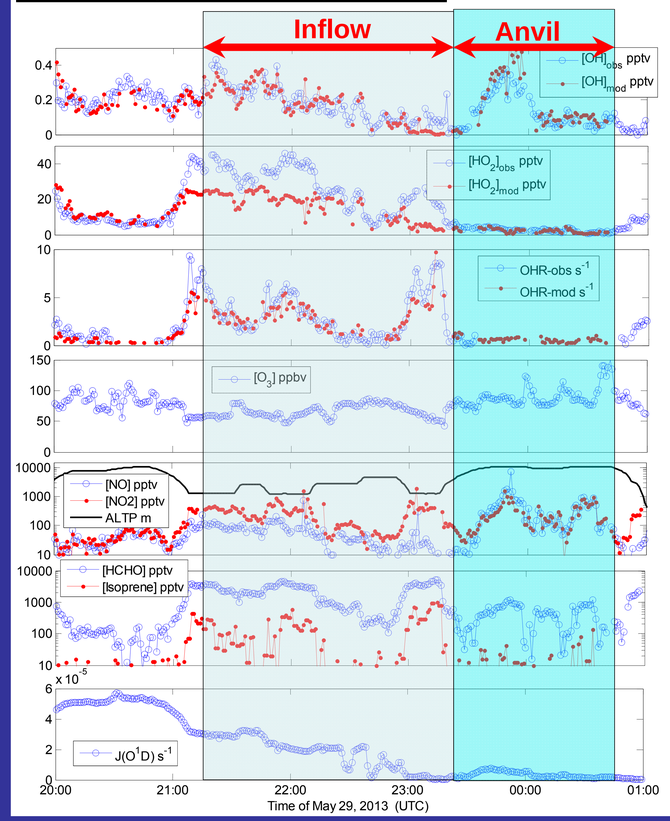


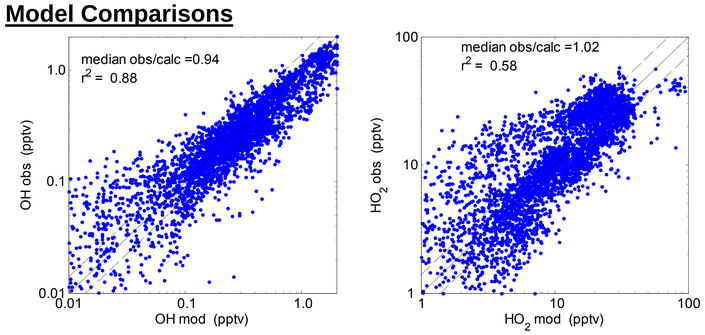
Fig. 4 Flight track color-coated with HO_2 mixing ratio during DC3.

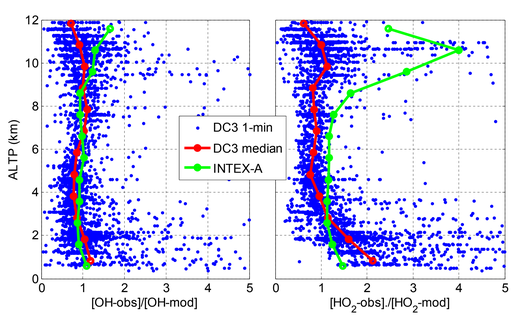
- Relatively constant [OH] between 2-10 km and elevated [OH] above 10 km.
- [HO_2] decreases as altitude increases.
- Higher OH and HO_2 levels during INTEX-A (July 2004) than during DC3 (May-June, 2012) due to lower solar radiation during DC3, but similar HO_2/OH ratios in the two studies.
- OH reactivity (OHR): elevated in BL and generally low in the FT. Good agreement with a median obs-to-calc ratio of 1.10. CO, NMHC, and OVOCs are main OHR contributors.
- Significant OHR (3-5 s^{-1}) in some outflows was observed.

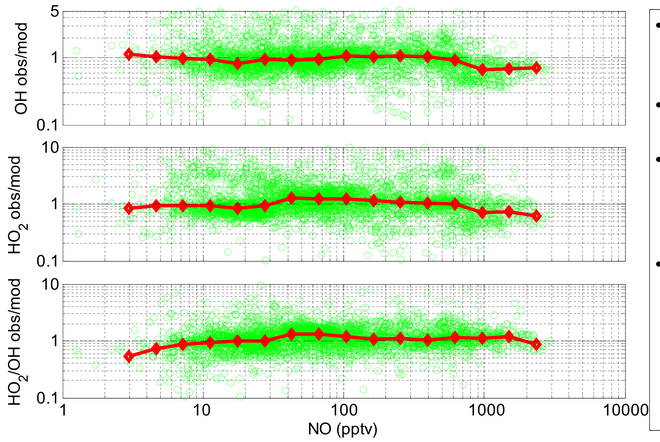
A case Study on 5/29/2012 (OK Storm)



Model Comparisons

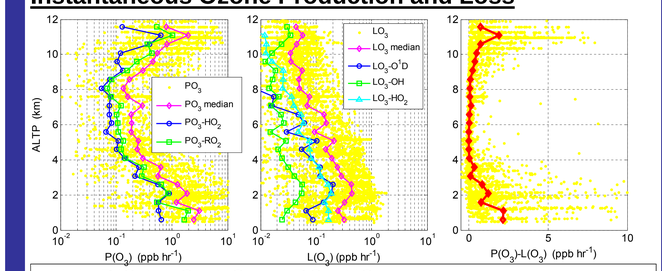






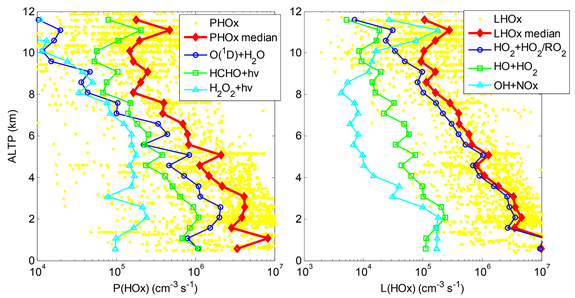
- In general, measured OH and HO_2 agree well with the model calculations within the combined measurement and model uncertainty.
- On average, the model tends to under-predict HO_2 at low altitudes.
- No significant NO dependence in observed-to-modeled OH and HO_2 ratios. The ratios are slightly less than unit when NO levels were greater than 1 ppbv indicating model over-prediction of OH and HO_2.
- Compared to INTEX-A:
  - OH ratio: similar @ 0-10km, slightly < 1 @ >10km during DC3; slightly > 1 @ >10km during INTEX-A
  - HO_2 ratio: significantly > 1 @ >8km during INTEX-A; >1 @ < 2km in both studies

Instantaneous Ozone Production and Loss



- Main $P(O_3)$: HO_2+NO and RO_2+NO
- Main $L(O_3)$: O_3+HO_2 and $O(^1D)$+H_2O
- Net $P(O_3)$: close to zero between 4-10km; a few ppb h^{-1} in UT/BL

HO_x Budget



Main $P(HO_x)$: $O(^1D)$ + H_2O @ < 7 km HCHO+hv @ >8 km

Main $L(HO_x)$: HO_2+HO_2/RO_2 @ < 10 km; OH + NO_x @ > 10 km

Summary

- OH, HO_2, and OH reactivity were successfully measured on the NASA DC-8 during DC3.
- A box model based RACM2 was able to reproduce OH and HO_2 generally well, with a median observed-to-modeled ratio of 0.94 for OH and 1.02 for HO_2, although the model tends to under-predict HO_2 at low altitudes.
- No significant NO dependence in obs-to-mod OH and HO_2 ratios, although the model tends to slightly under-predict both OH and HO_2 when NO levels were greater than 1 ppbv.
- Good agreement between the observed and calculated OH reactivity, with a median obs-to-calc ratio of 1.10. CO, NMHC, and OVOCs dominated OH reactivity.
- In an Oklahoma storm survey on May 29, 2012, the box model was able to simulate OH well but under-predicted HO_2 in inflow. Excellent agreement was obtained between observed and calculated OH reactivity.
- Main $P(HO_x)$ was $O(^1D)$+H_2O below 7 km and HCHO+hv above 8 km. Main $L(HO_x)$ was HO_2+HO_2/RO_2 below 10 km and OH + NO_x above 10 km .
- A net O_3 production of a few ppbv hr^{-1} below 2 km and above 10 km was observed.

Acknowledgements

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