An Initial Look at Testing Photochemical Theory During INTEX

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Purpose:

Characterize the relationship between measurements and photochemical theory

Ultimate Goals:

Seek to understand differences between observations and expectations based on current knowledge

Estimate the contribution of photochemistry to the observed ozone distribution

Assess the impact of convection on chemical processing in the upper troposphere

Assess the impact of NMHCs on ozone and oxidant levels
Time-dependent photochemical box model

Detailed HO\textsubscript{x}-NO\textsubscript{x}-CH\textsubscript{4}-NMHC mechanism

Constrained by observations: 
T, P, H\textsubscript{2}O, O\textsubscript{3}, CO, NO, non-methane hydrocarbons, acetone, photolysis rates

When observations are available, additional model constraints include: 
H\textsubscript{2}O\textsubscript{2}, CH\textsubscript{3}OOH, HNO\textsubscript{3}, PAN, HCOOH, CH\textsubscript{3}COOH

Predicted species: 
OH, HO\textsubscript{2}, RO\textsubscript{2}, CH\textsubscript{2}O, H\textsubscript{2}O\textsubscript{2}, CH\textsubscript{3}OOH, ROOH, NO\textsubscript{2}, HNO\textsubscript{3}, PAN, ROOH, etc.

Calculated species are integrated in time until diurnal profile converges.

NO\textsubscript{x} held constant, but partitioning varies throughout the diurnal cycle

Diurnal variation of photolysis rates from TUV (DISORT 8 streams)
Model-Measurement Comparison of NO (Brune)

NO calc > 100 pptv
Model-Measurement Comparison of HO2 (Brune)
Model-Measurement Comparison of H2O2 (Heikes)
Model-Measurement Comparison of HO2NO2 (Huey)
Model-Measurement Comparison of CH2O (Fried)
Trends in Model-Measurement Agreement with NO
Trends in Model-Measurement Agreement with NO
Trends in Model-Measurement Agreement with NO
Trends in Model-Measurement Agreement with NO

- HO2 and sqrt(H2O2) and HO2NO2 calc/obs

- Trends in Model-Measurement Agreement with NO
Trends in Model-Measurement Agreement with Isoprene
Trends in Model-Measurement Agreement with Isoprene

![Graph showing trends in model-measurement agreement with isoprene.

The graph plots Isoprene (ppbv) against OH calc/obs. The data points are color-coded to represent Isoprene chemistry and No Isoprene chemistry. The graph highlights the agreement between model calculations and observational data.]
Trends in Model-Measurement Agreement with NO Isoprene chemistry

No Isoprene chemistry
Summary

INTEX offers an unprecedented number of measurements suitable for testing photochemical theory.

Comparisons are somewhat paradoxical.

Current estimated ozone production rates for the upper troposphere are 4-5 ppbv/day (could it be closer to 10 ppbv/day!?)

Input from the Science Team regarding these and other applications of the model are welcomed.