An Initial Look at Testing Photochemical Theory During INTEX



Jim Crawford, Gao Chen, Jennifer Olson, and Margaret Pippin

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_x-NO_x-CH₄-NMHC mechanism

Constrained by observations:

T, P, H₂O, O₃, CO, NO, non-methane hydrocarbons, acetone, photolysis rates

When observations are available, additional model constraints include: H_2O_2 , CH_3OOH , HNO_3 , PAN, HCOOH, CH_3COOH

Predicted species:

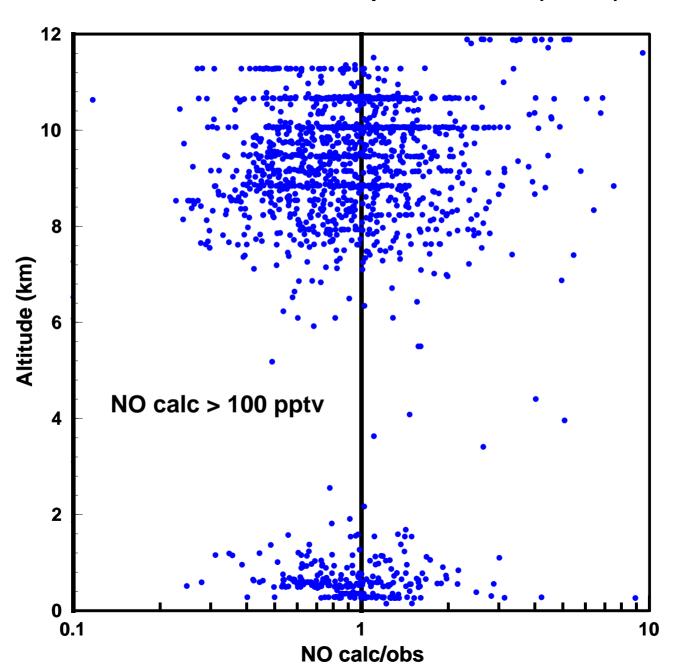
OH, HO₂, RO₂, CH₂O, H₂O₂, CH₃OOH, ROOH, NO₂, HNO₃, PAN, ROOH, etc.

Calculated species are integrated in time until diurnal profile converges.

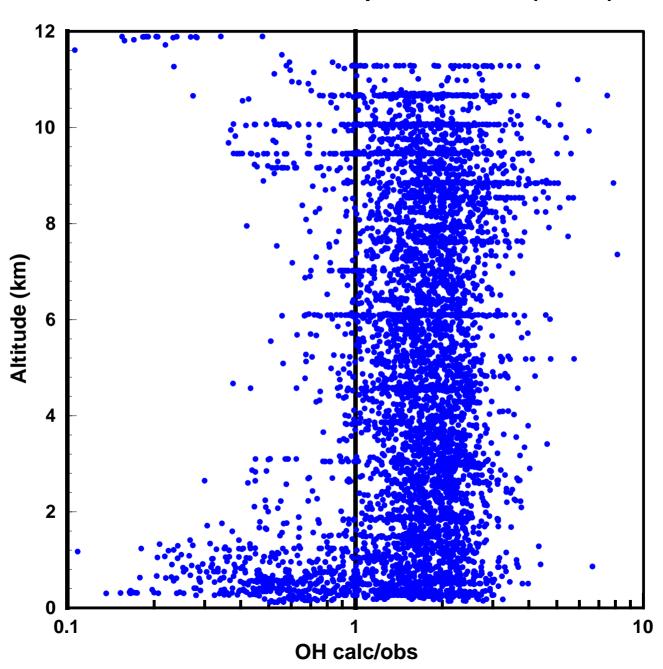
NO_x held constant, but partitioning varies throughout the diurnal cycle

Diurnal variation of photolysis rates from TUV (DISORT 8 streams)

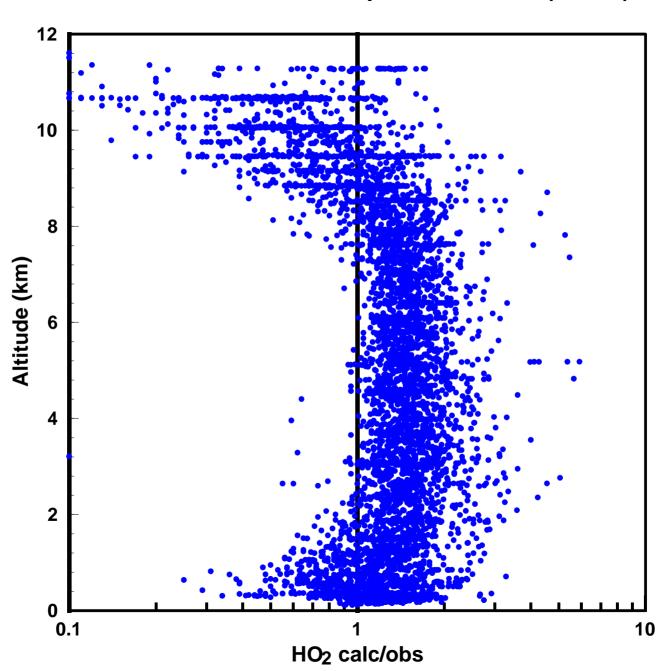
Model-Measurement Comparison of NO (Brune)



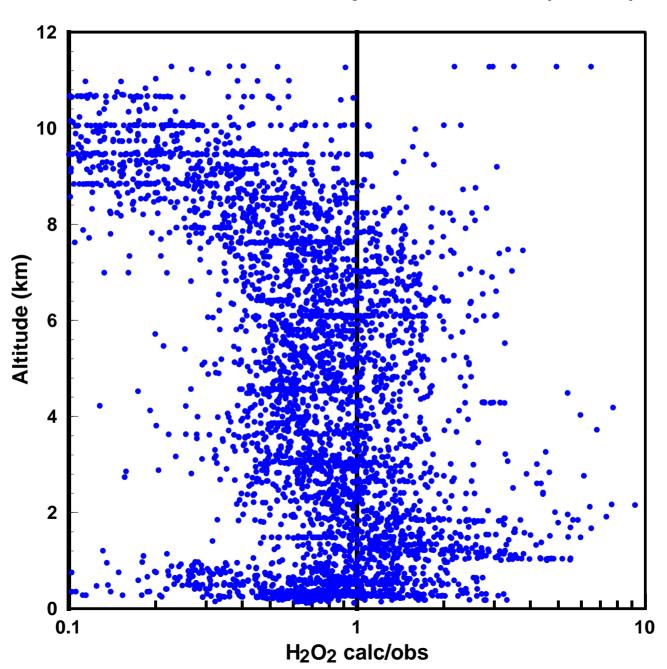
Model-Measurement Comparison of OH (Brune)



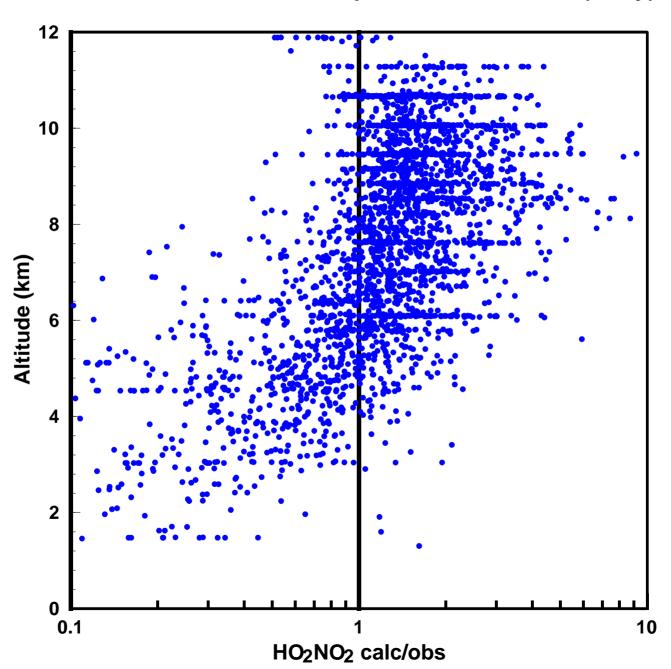
Model-Measurement Comparison of HO2 (Brune)



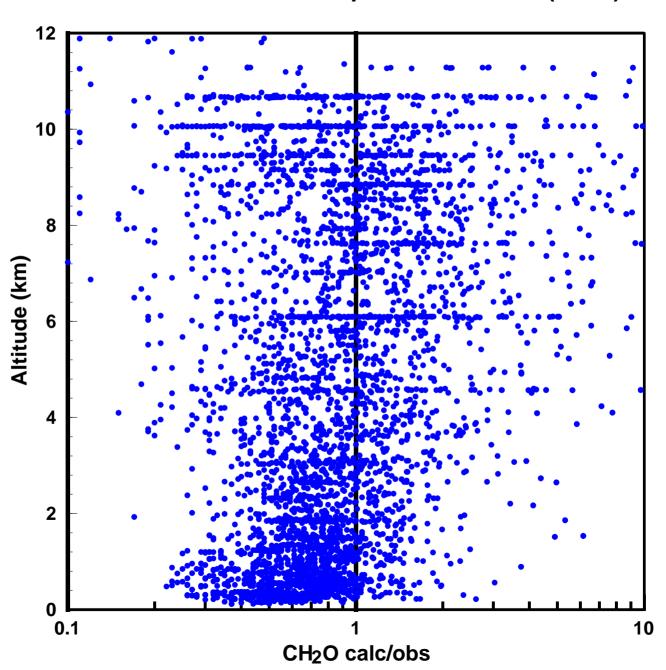
Model-Measurement Comparison of H2O2 (Heikes)

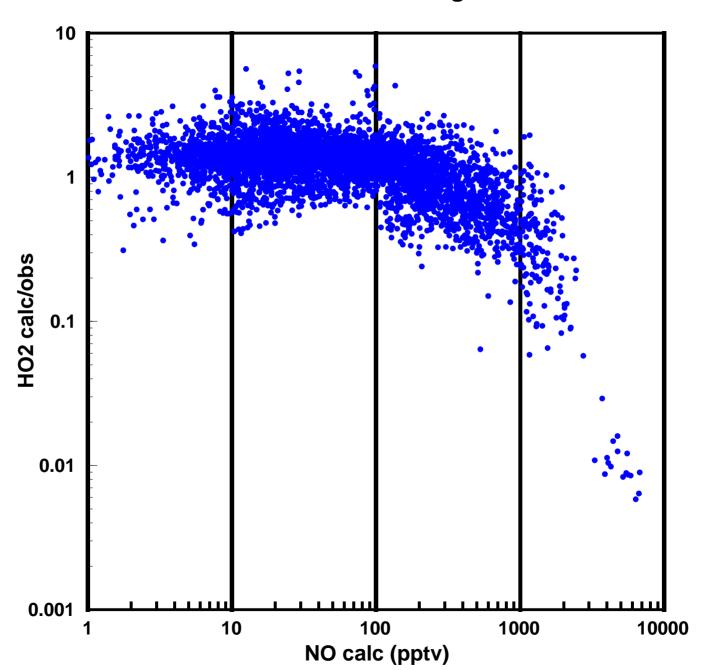


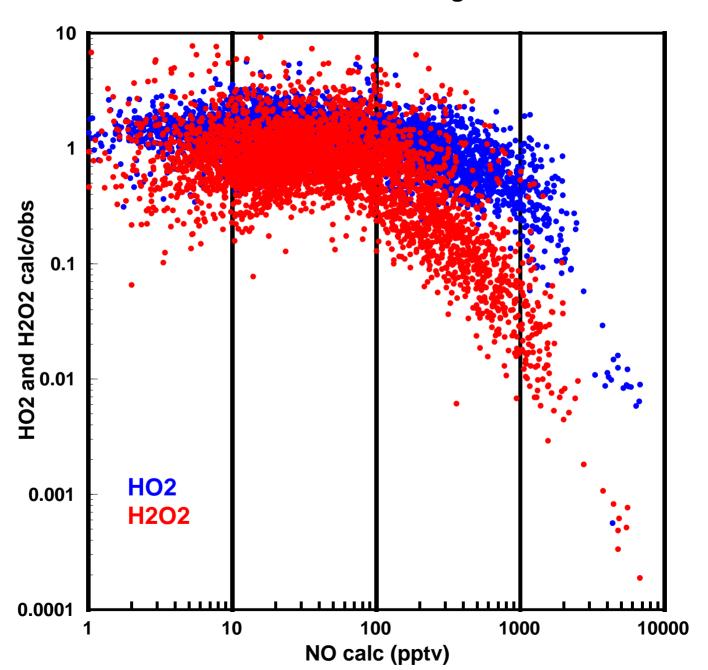
Model-Measurement Comparison of HO2NO2 (Huey)

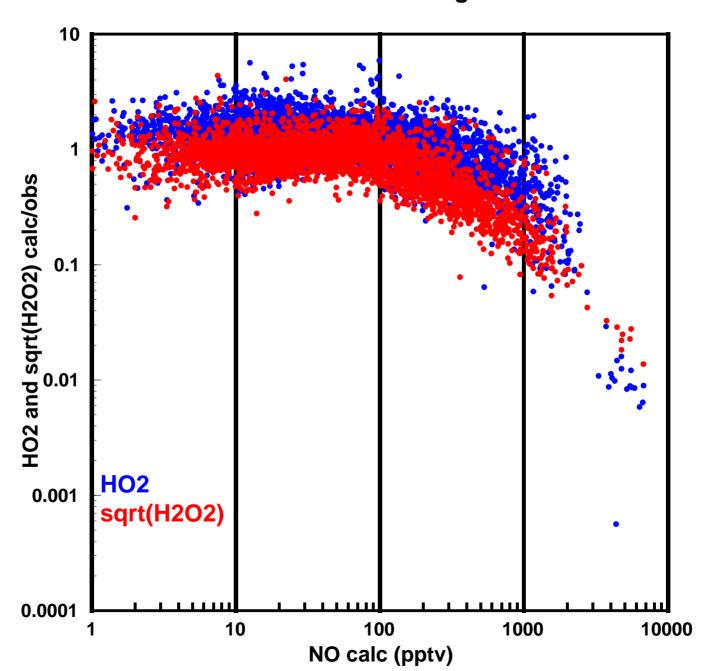


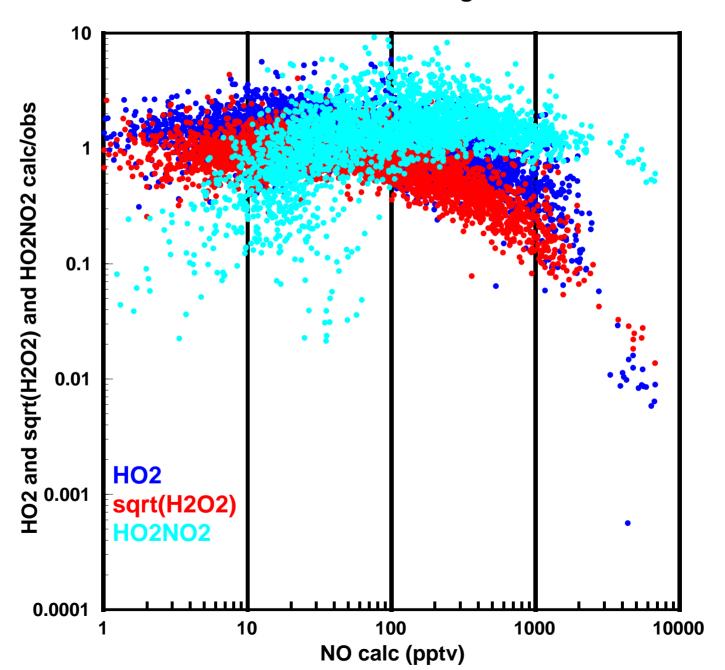
Model-Measurement Comparison of CH2O (Fried)



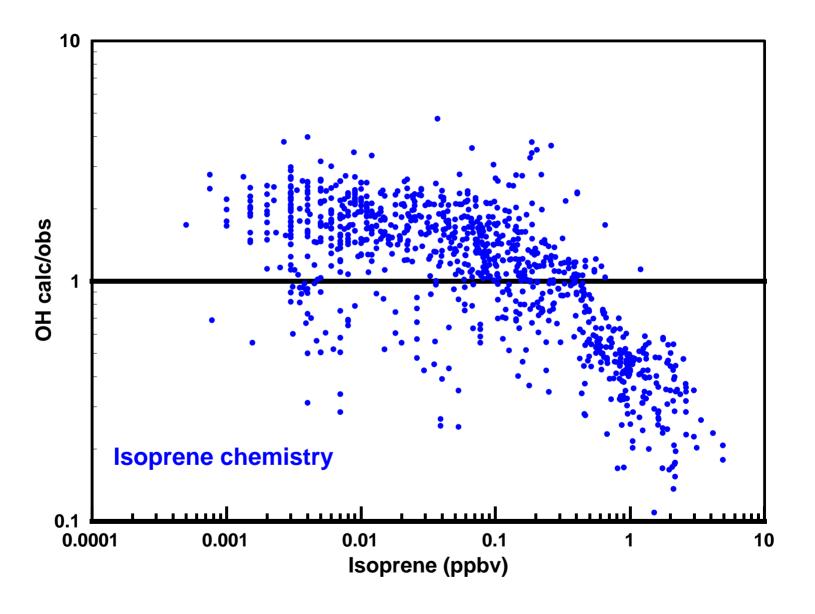




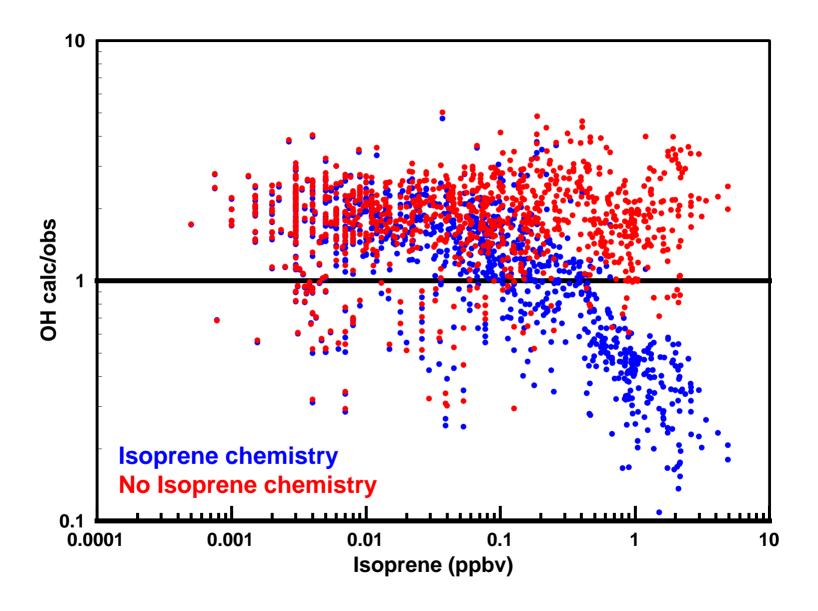


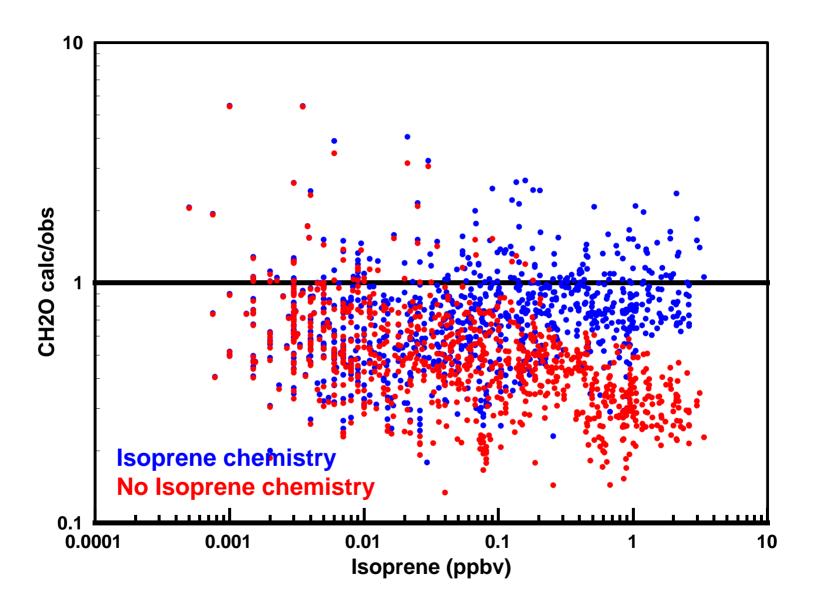


Trends in Model-Measurement Agreement with Isoprene



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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.