MOZART Photochemistry and Transport Modeling for ICARTT

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MOZART Chemical Transport Model

Chemistry
- ~100 gas and aerosol species, ~200 reactions
- Tagged fossil fuel and biomass CO from 9 continental source regions
- Output every 3 hours, sampled along flight tracks

Meteorology
- NCEP Reanalysis*
- NCEP Global Forecast System (GFS)

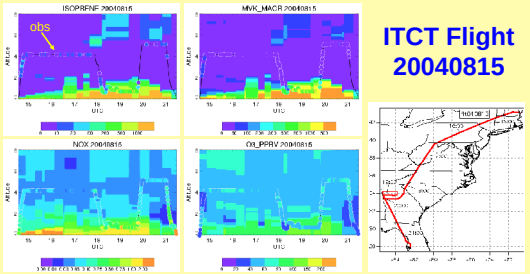
Resolution
- 1.9° latitude x1.9° longitude x 28 vertical levels*
- 1.4° latitude x1.4° longitude x 64 vertical levels

Fossil Fuel Emissions
- ICARTT surface emissions (N. America), EDGAR (elsewhere)

Biomass Burning Emissions
- Climatological*
- Daily observed burning from MODIS and NICC (Turquety and Hudman, Harvard)

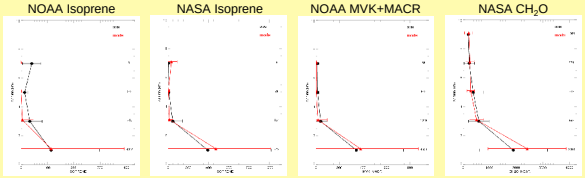
* Default values used in this poster unless otherwise indicated

Isoprene Chemistry in the Southeast US



ITCT Flight 20040815

Mission Summary

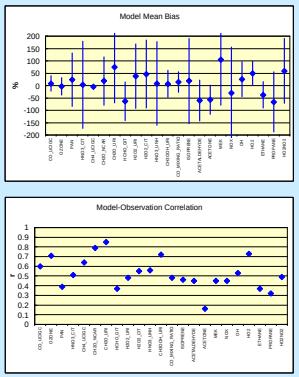


Hydrocarbon reactivity in the southeastern U.S. is dominated by isoprene. We plan to use the suite of measurements available from ICARTT to help constrain uncertainties in isoprene emissions (currently a factor of 2-3) and its oxidation chemistry (*e.g.* isoprene nitrates, formaldehyde, ozone). Our initial evaluation shows:

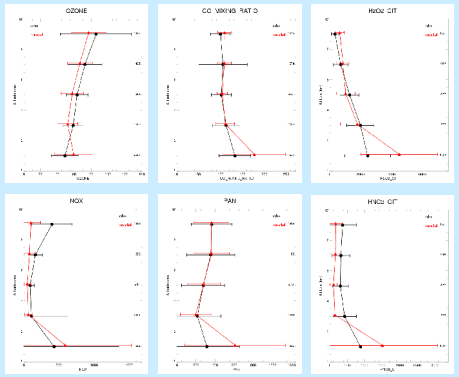
- Good agreement of isoprene and oxidation products (MVK+MACR, CH_2O) with observations
- Discrepancies in HO_x radical concentrations (OH and HO_2 too high by 30-50%), which affect the sensitivity of ozone to isoprene

Comparison of Model Results and Observations

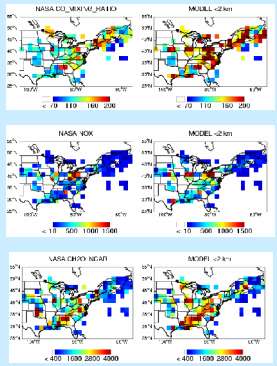
Model Bias and Correlation vs. All INTEX DC-8 Observations



Mean Vertical Profiles Model vs. INTEX DC-8 Observations



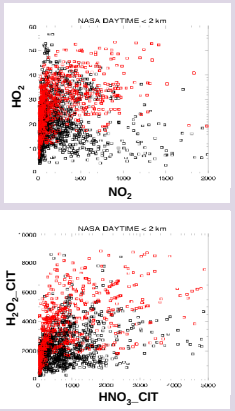
Model vs. INTEX Observations Lower Troposphere (< 2km), Daytime



SUMMARY

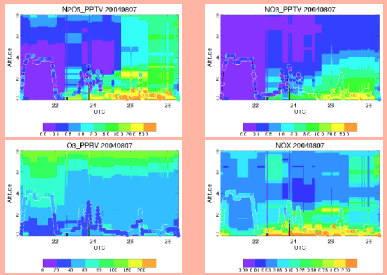
- **Model captures O_3, CO, NO_x, PAN, H_2O_2 observations in free troposphere, but is biased high in continental boundary layer**
- **Underestimate of hydrocarbons (ethane by ~40%, propane by ~60%) and oxidation products (acetaldehyde by ~100 pptv, acetone by ~1 ppbv)**
- **HNO_3 biased high in boundary layer, but low in free troposphere**

Ozone Chemical Regime Model vs. Observations



The ratio HO_2 : NO_2 controls the sensitivity of ozone production to NO_x vs. VOC emissions. The observed H_2O_2 : HNO_3 ratio has been used as a proxy for the ozone production regime. The model is more HO_x-rich (*i.e.*, NO_x-sensitive) and also shows a stronger HO_x-NO_x correlation than observed.

Nighttime Chemistry



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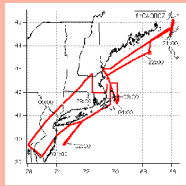

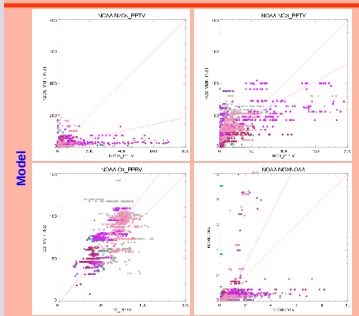

All ITCT Night Flights

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20040731
20040803
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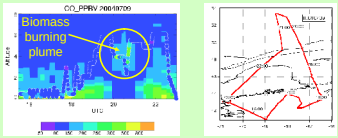
20040809
20040811

- **Typical concentrations of N_2O_5 and NO_3 captured to within 50%**
- **Errors in N_2O_5 are related to errors in NO_x, likely associated with poor representation of subgrid-scale urban plumes**

Future Work

- Analyze impacts of biomass burning on background chemistry



(Using observed biomass burning)

- Investigate source of continental boundary layer biases
- Intercontinental transport
  - –Asia → North America
  - –North America → Europe
- MOZART output fields available by request from **Larry Horowitz** or **Arlene Fiore**